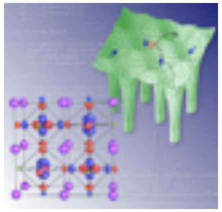
Excitonic magnetism in models and materials

Jan Kuneš

Collaborators

Pavel Augustinský	IoP Prague
Dominique Geffroy	Masaryk University Brno
Vladislav Pokorný	Uni. Augsburg + IoP Prague
Pavel Novák	IoP Prague
Jindřich Kolorenč	IoP Prague
Karel Pajskr	Charles University, Prague
Ryotaro Arita	RIKEN, Tokyo



DFG Research Unit FOR1346

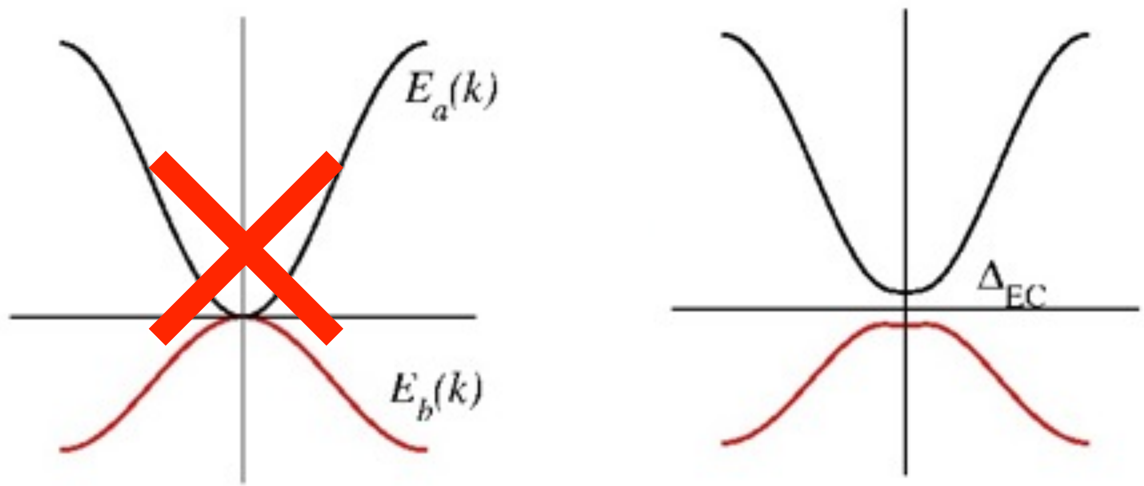
Czech Science Foundation

European Research Council

Excitonic insulator

"The first point that we must make about this model is that the predicted continuous increase in the number of free electrons and holes from the value zero is not possible. An electron and a positive hole will attract each other … the electron and hole will always, when in the state of lowest energy, form pairs (excitons) …"

Neville Mott, 1961



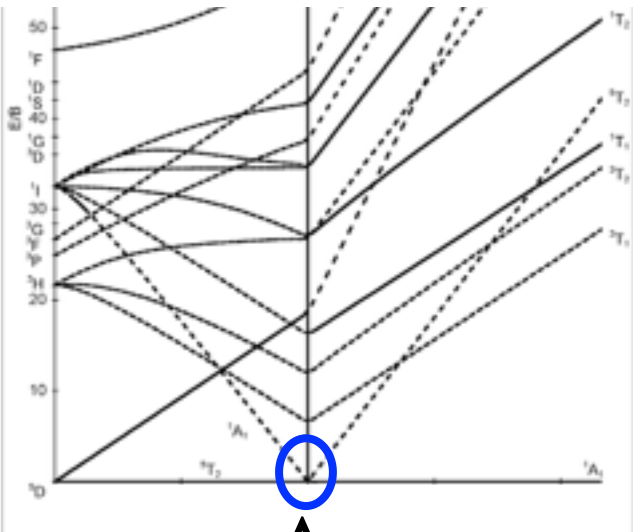
Knox, 1963
Keldysh and Kopaev, 1965
des Cloizeaux, 1965
Kozlov and Maksimov, 1966
Jerome, Rice, Kohn 1967
Halperin and Rice, 1968

} weak coupling BCS like theories

Spin-state transition

Spin-state transition is a rapid change of magnitude or disappearance of the fluctuating local moment.

Ligand field physics
(single atom)

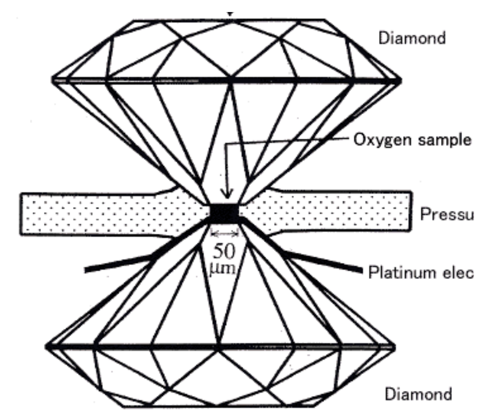


Δ_{CF}

Tanabe & Sugano, 1954

- compounds containing Mn, Fe, Co

- high pressures (~ 10 GPa)
  Earth mantle or diamond anvil cell



- as a function of temperature, strain, …
  $LaCoO_3$

Outline

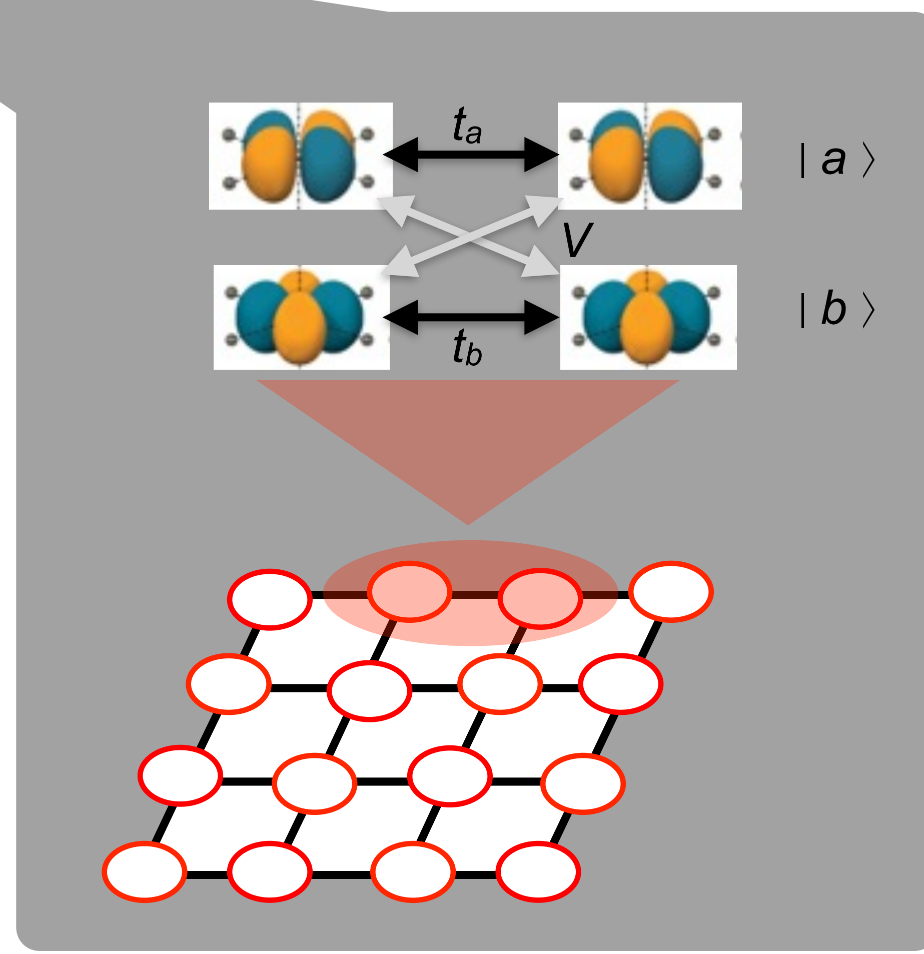
- Two-band Hubbard model
  - Strong-coupling limit (hard-core bosons)
  - Dynamical mean-field theory (fermions)
  - Exotic properties - spin texture

- Real materials $(Pr_xR_{1-x})_yCa_{1-y}CoO_3$ (PCCO) and Sr_2YIrO_6
  - Excitonic condensation with orbital degeneracy
  - Density functional theory (LDA+U)

Excitonic condensation in Hubbard model

Two-band Hubbard model at n=2 (half filling)

$$H_{\mathrm{t}} = \frac{\Delta}{2}\sum_{i,\sigma}(n^a_{i\sigma} - n^b_{i\sigma}) + \sum_{i,j,\sigma}(t_a a^\dagger_{i\sigma} a_{j\sigma} + t_b b^\dagger_{i\sigma} b_{j\sigma})$$
$$+ \sum_{\langle ij\rangle,\sigma}(V_1 a^\dagger_{i\sigma} b_{j\sigma} + V_2 b^\dagger_{i\sigma} a_{j\sigma} + c.c.)$$
$$H^{\mathrm{dd}}_{\mathrm{int}} = U\sum_i (n^a_{i\uparrow} n^a_{i\downarrow} + n^b_{i\uparrow} n^b_{i\downarrow}) + (U-2J)\sum_{i,\sigma} n^a_{i\sigma} n^b_{i-\sigma}$$
$$+ (U-3J)\sum_{i\sigma} n^a_{i\sigma} n^b_{i\sigma}$$
$$H'_{\mathrm{int}} = J\sum_{i\sigma} a^\dagger_{i\sigma} b^\dagger_{i-\sigma} a_{i-\sigma} b_{i\sigma} + J'\sum_i (a^\dagger_{i\uparrow} a^\dagger_{i\downarrow} b_{i\downarrow} b_{i\uparrow} + c.c.).$$



John Hubbard

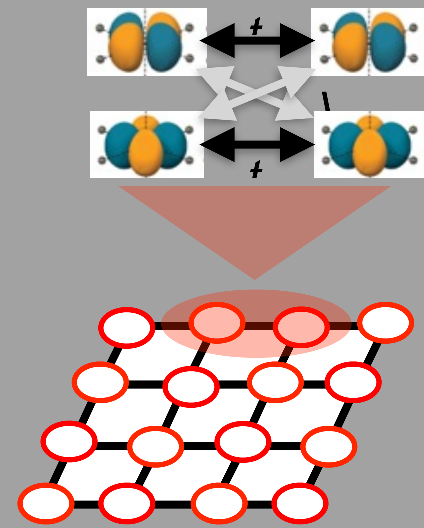
Proximity to spin-state crossover

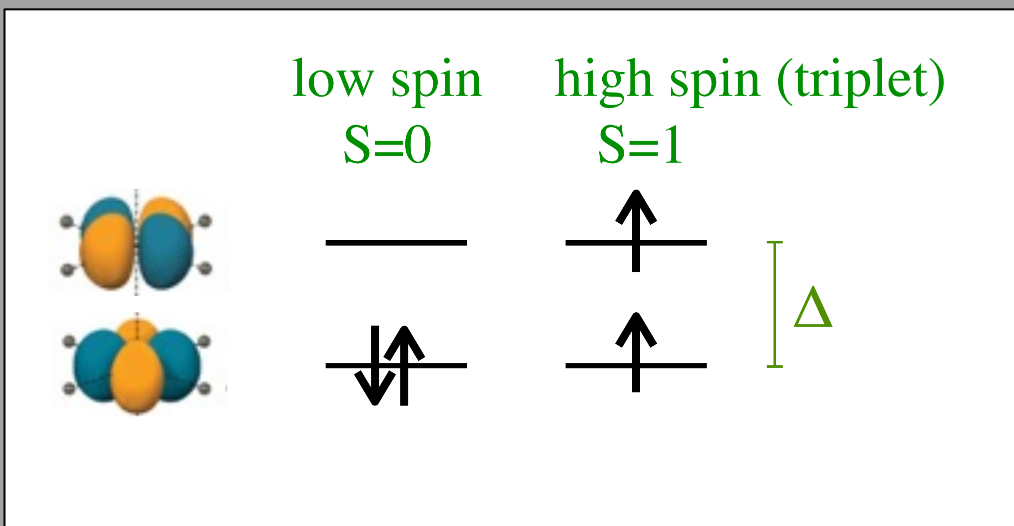
Two-band Hubbard model at n=2 (half filling)

$$H_{\rm t} = \frac{\Delta}{2}\sum_{i,\sigma}(n^a_{i\sigma} - n^b_{i\sigma}) + \sum_{i,j,\sigma}(t_a a^\dagger_{i\sigma} a_{j\sigma} + t_b b^\dagger_{i\sigma} b_{j\sigma})$$

$$+ \sum_{\langle ij\rangle,\sigma}(V_1 a^\dagger_{i\sigma} b_{j\sigma} + V_2 b^\dagger_{i\sigma} a_{j\sigma} + c.c.)$$

$$H^{\rm dd}_{\rm int} = U\sum(n^a_{i\uparrow}n^a_{i\downarrow} + n^b_{i\uparrow}n^b_{i\downarrow}) + (U-2J) \ldots n^b_{i-\sigma}$$





Competition of Hund’s coupling *J* and crystal-field Δ

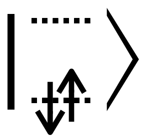
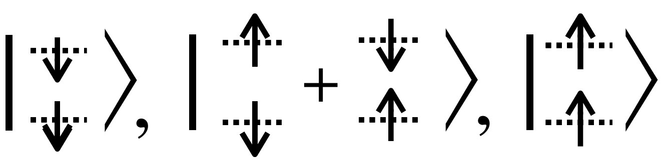
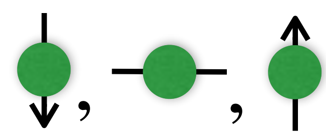
We are interested in $E_{LS} \simeq E_{HS}$

Strong-coupling limit
(hard-core bosons)

Strong coupling theory

Balents 2000
Rademaker et al. 2012-2014
bilayer Heisenberg model

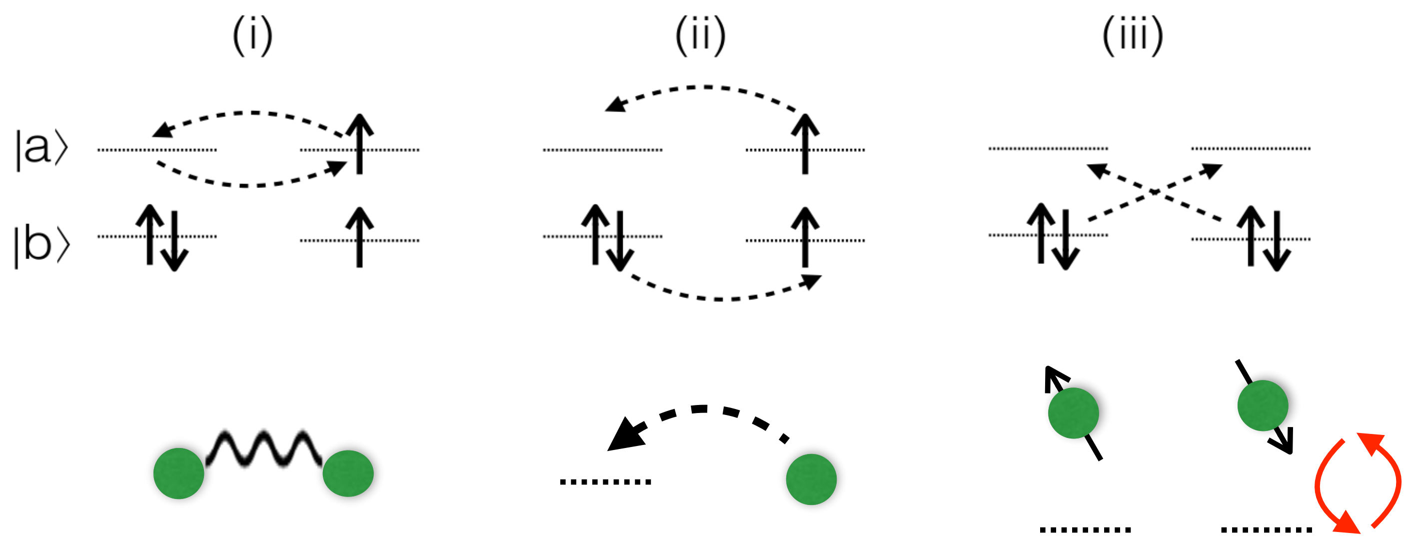
- Define restricted low-energy Hilbert space

Fermions	Bosons (hard-core)
low-spin state 	vacuum
high-spin state 	S=1 boson 
LS -> HS transition $a^\dagger_\downarrow b_\uparrow\,, \ldots$	creation of a boson $d^\dagger_{-1}\,, \ldots$

Strong coupling theory

- Decouple it from the high-energy states (Schrieffer-Wolff transformation)

Typical 2nd order processes:



Effective Hamiltonian:

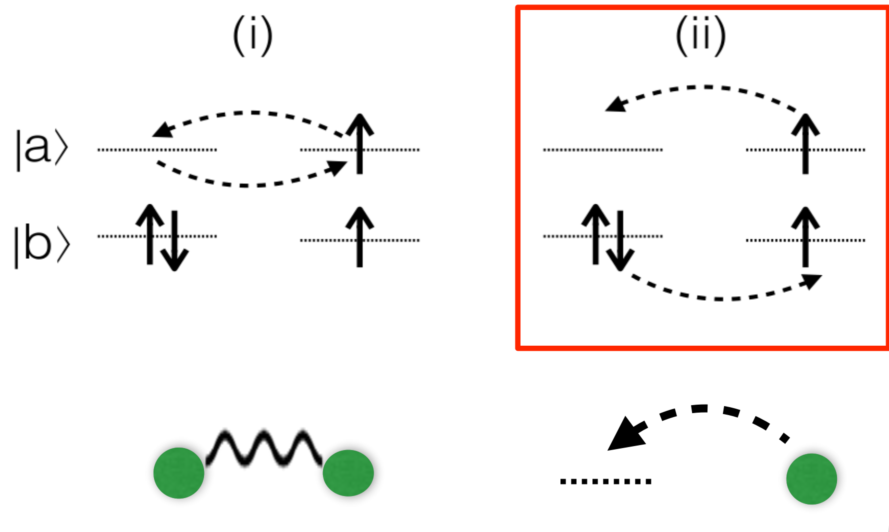
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) +$$

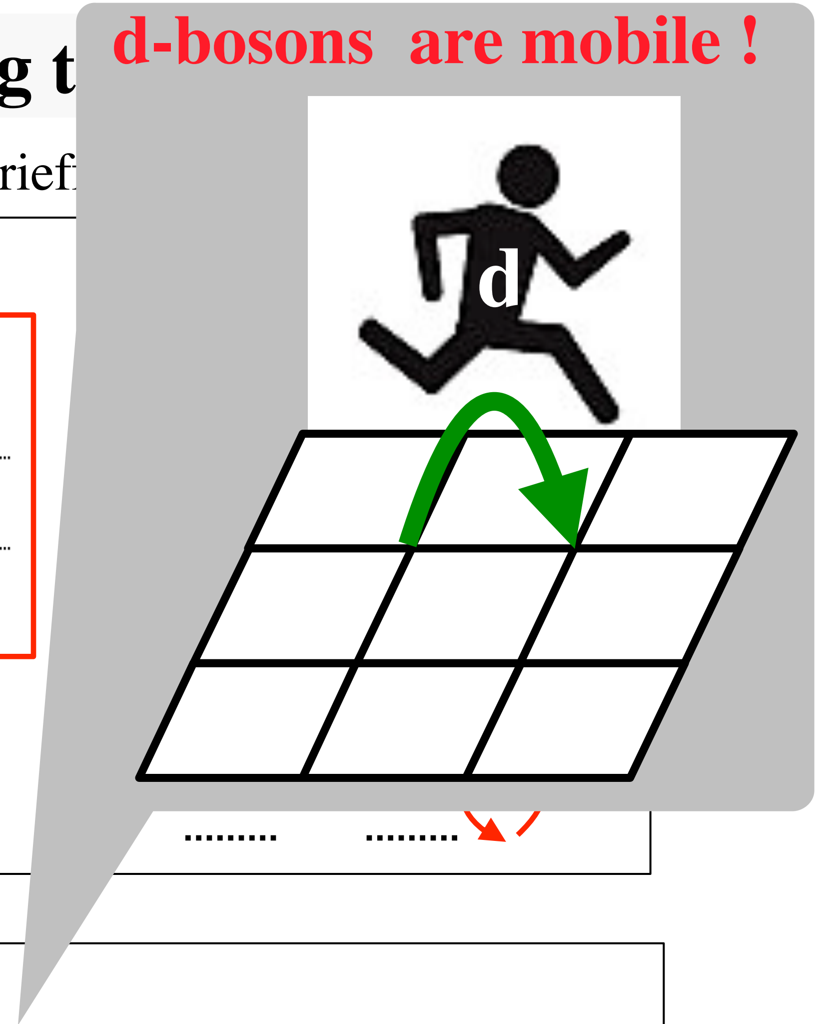
$$K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K_1 \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j^\dagger + H.c. \right) + \ldots$$

Strong coupling t

- Decouple it from the high-energy states (Schrief

Typical 2nd order processes:





Effective Hamiltonian:

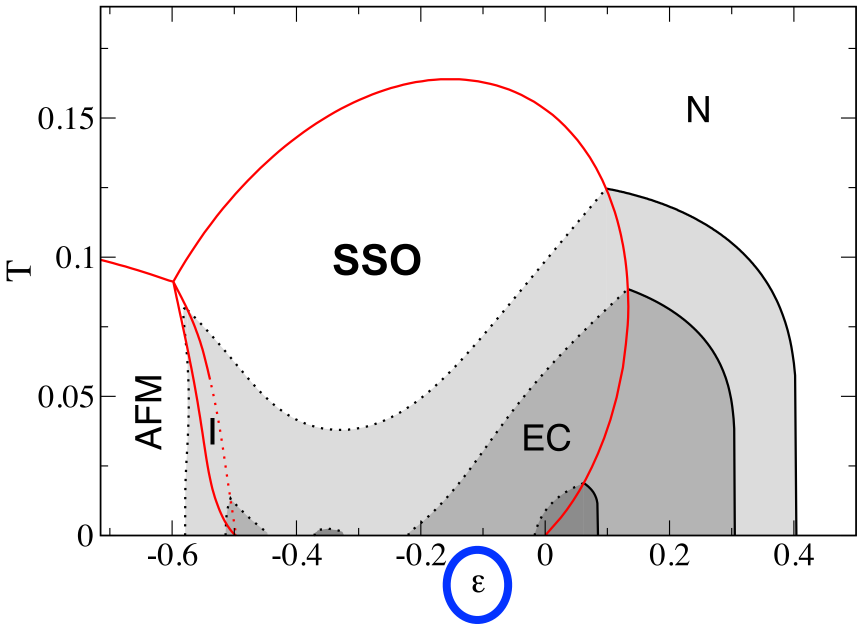
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) +$$

$$K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K_1 \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j^\dagger + H.c. \right) + \dots$$

Mean-field theory

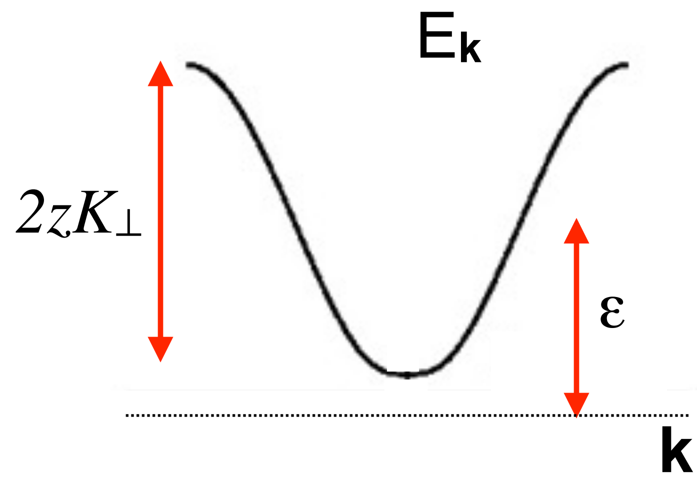
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

excitations in the normal state

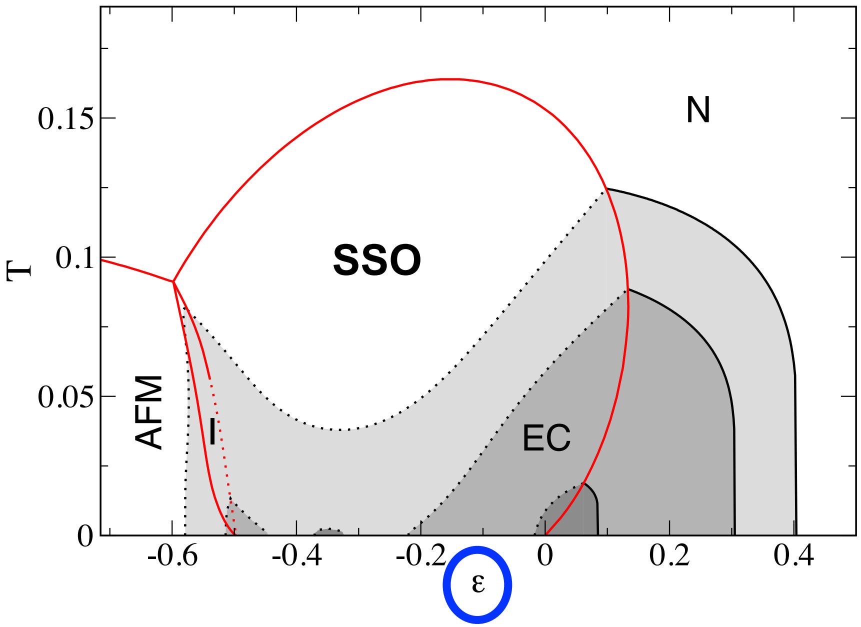


d-occupancy: $\langle n \rangle = 0$

Mean-field theory

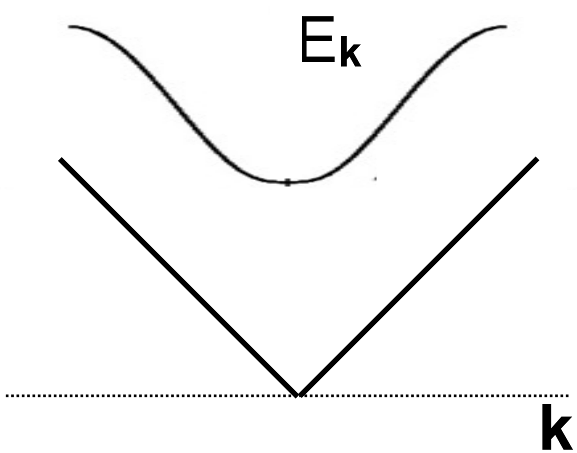
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

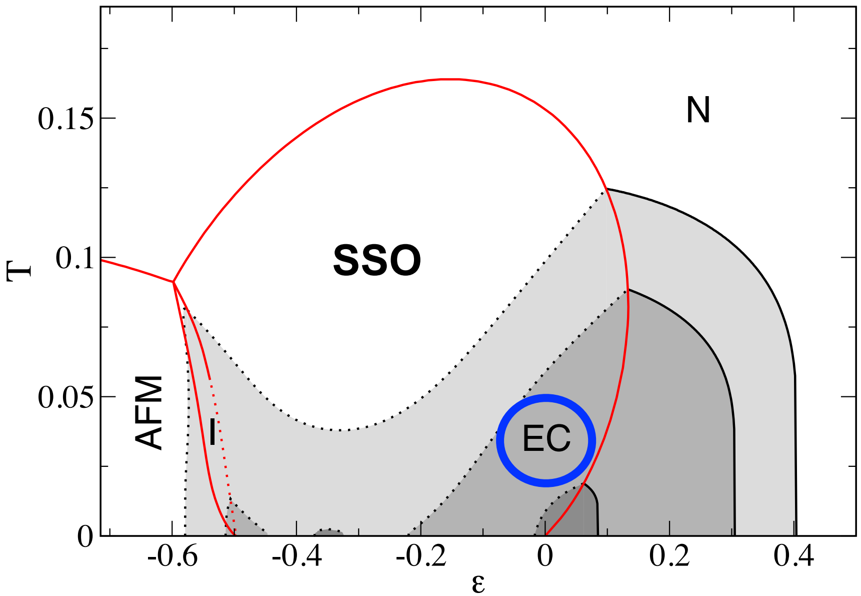
excitations of the condensate



Mean-field theory

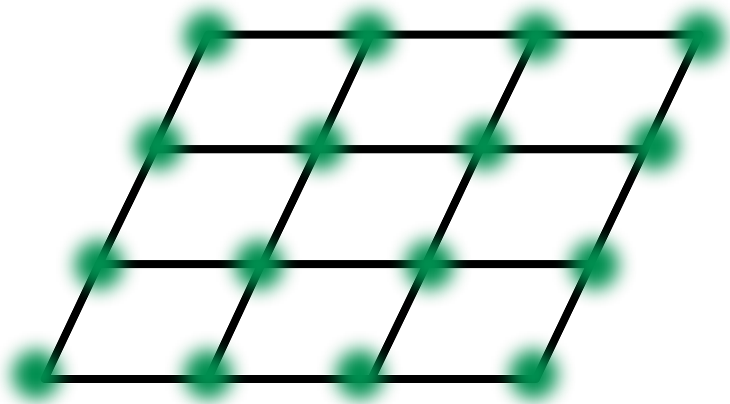
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

Bose-Einstein condensate of d-bosons



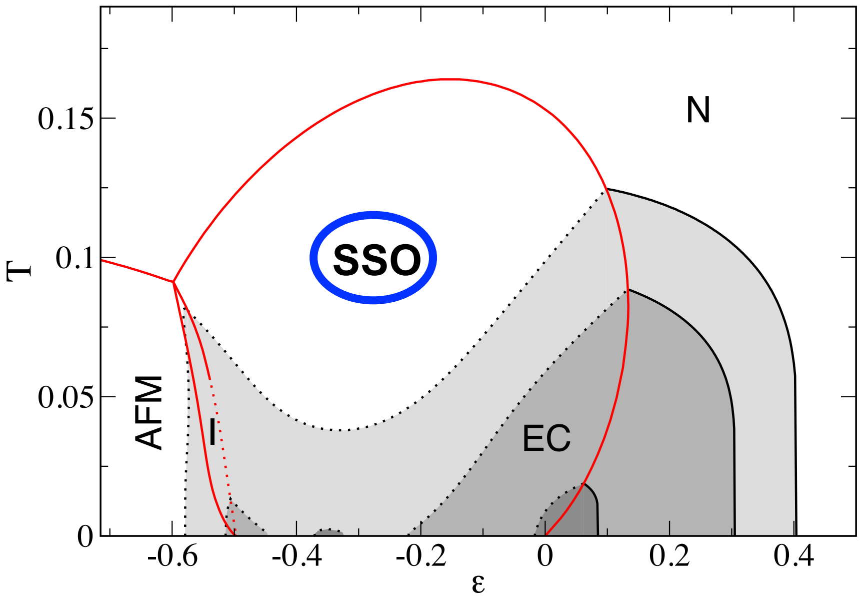
Order parameter: $\langle d_s \rangle$

d-occupancy: $0 < \langle n \rangle < 1$

Mean-field theory

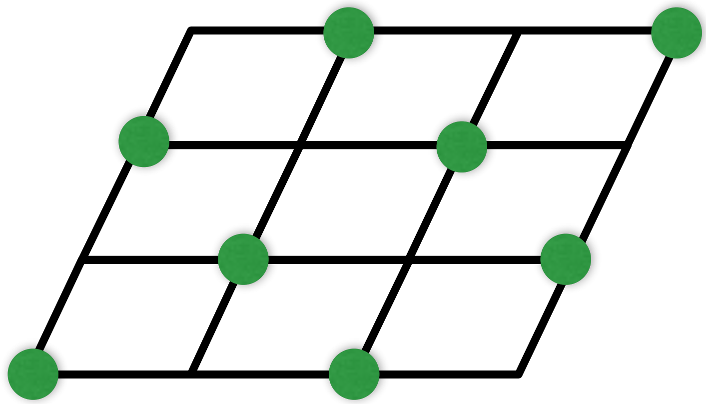
$$H_{\rm eff} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

Checkerboard spin-state order



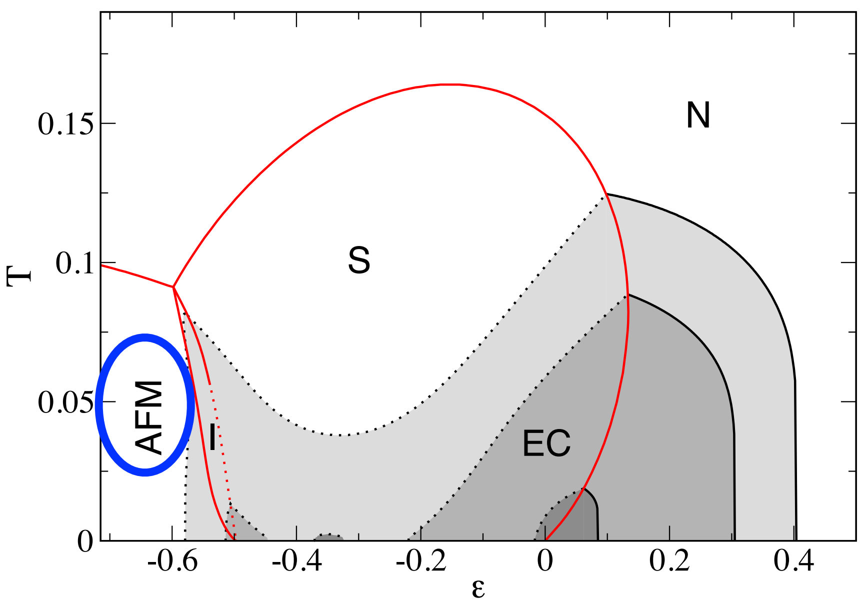
Order parameter: $\langle n_i - n \rangle$

d-occupancy: $\langle n \rangle = 1/2$

Mean-field theory

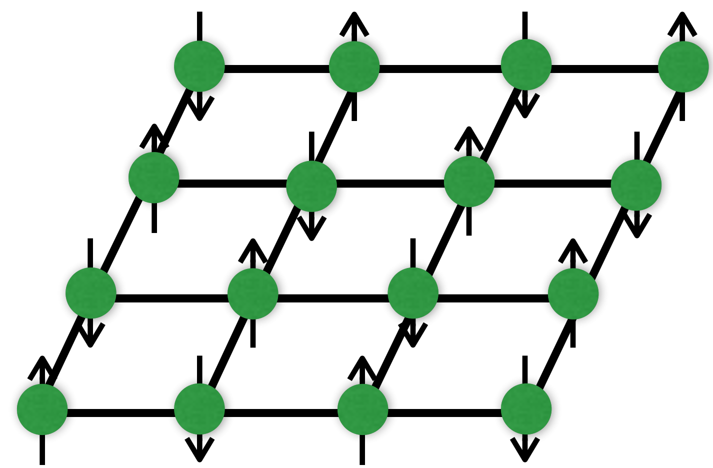
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

Heisenberg anti-ferromagnet



Order parameter: $\langle \mathbf{S}_i \rangle$

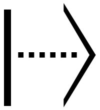
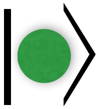
d-occupancy: $\langle n \rangle = 1$

What is exciton condensate?

Statistical mixture vs quantum superposition

What is exciton condensate?

Statistical mixture vs quantum superposition

Normal state - **statistical mixture** of  and 

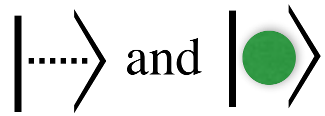
$$\langle d_s \rangle = 0$$

LS ground state + thermally populated HS states

$$\langle a_\sigma^\dagger b_{-\sigma} \rangle = 0$$

What is exciton condensate?

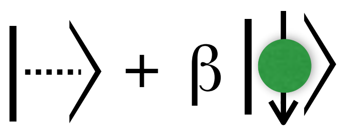
Statistical mixture vs quantum superposition

Normal state - **statistical mixture** of 

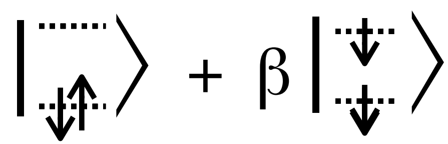
$$\langle d_s \rangle = 0$$

LS ground state + thermally populated HS states

$$\langle a^\dagger_\sigma b_{-\sigma} \rangle = 0$$

Condensate - **superposition** α 

$$\langle d_s \rangle \neq 0$$

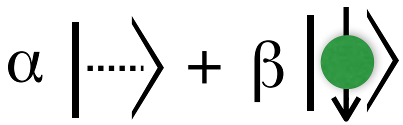
hybridised LS and HS states α 

$$\langle a^\dagger_\sigma b_{-\sigma} \rangle \neq 0$$

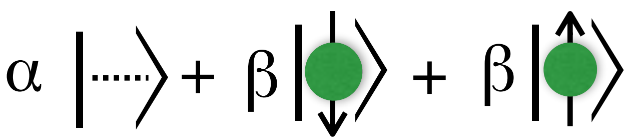
Condensate breaks symmetries of the Hamiltonian, e.g. spin rotation invariance

Boson degeneracy

Degenerate excitations -> distinct condensates possible



ferromagnetic condensate



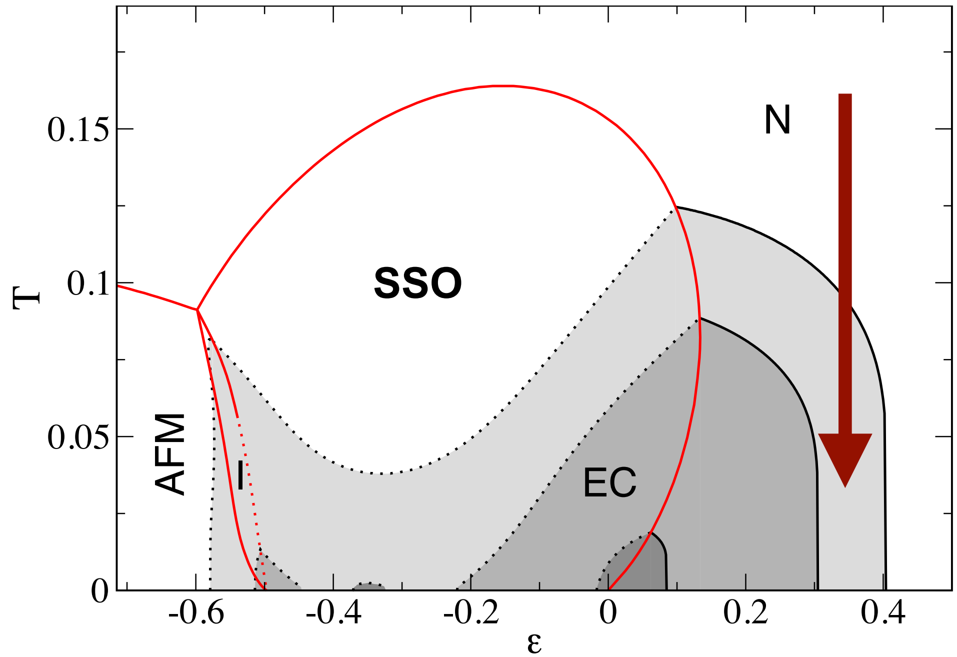
polar condensate

order parameter

$$\vec{\phi} = \sum_{\sigma,\sigma'} \langle a^\dagger_\sigma b_{\sigma'} \rangle \vec{\tau}_{\sigma\sigma'}$$

Back to fermions

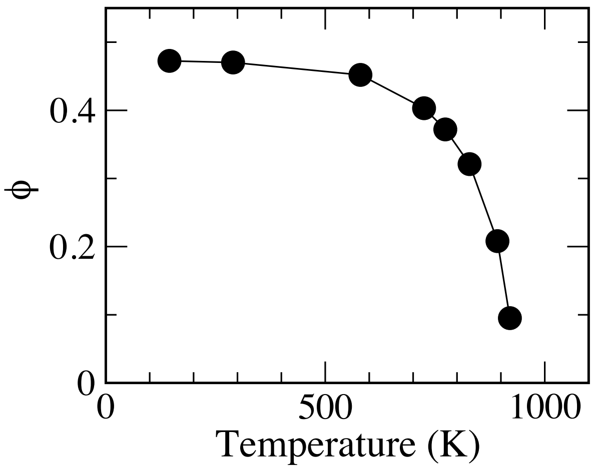
Numerical results (DMFT) excitonic instability:



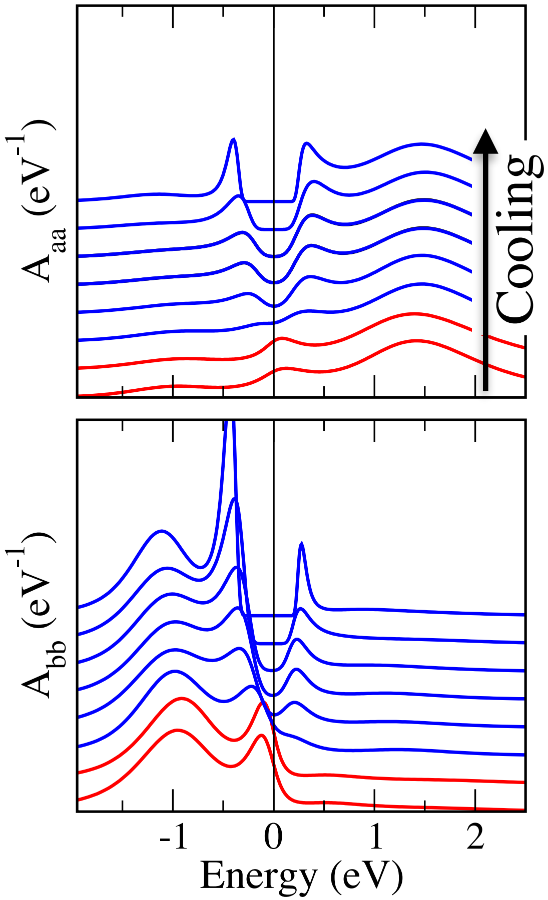
Undoped system - polar condensate

order parameter

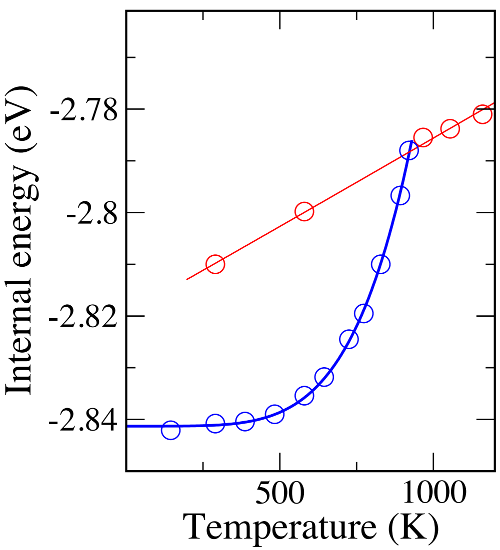
$$\phi = (\phi, 0, 0)$$

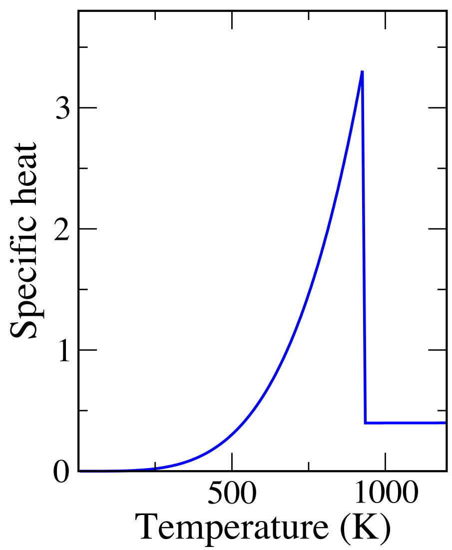


Spectral density (diagonal elements)



Internal energy and specific heat

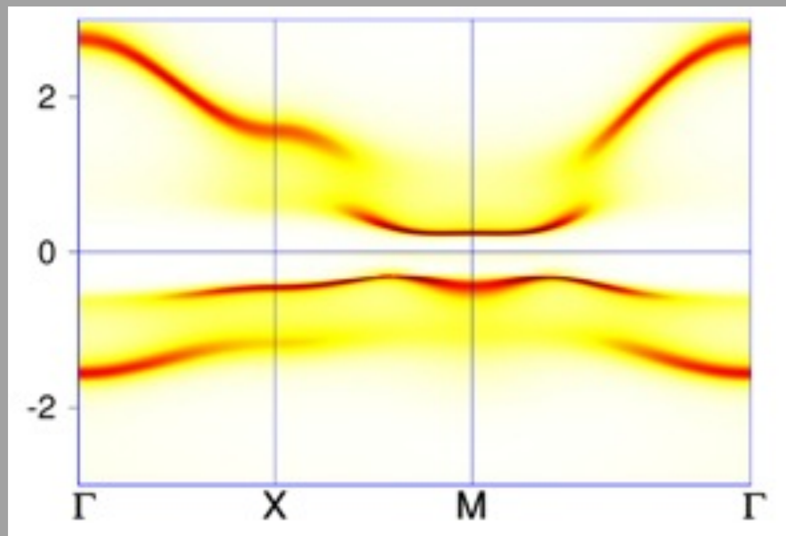




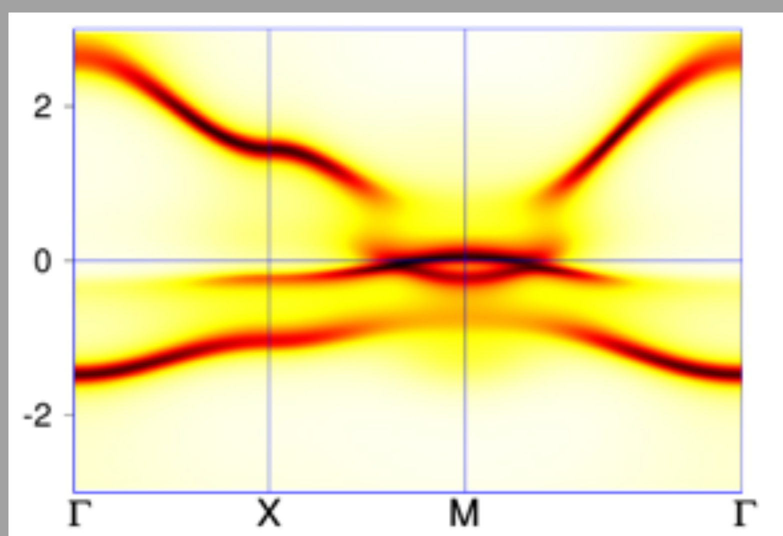
Undoped system - polar condensate

Opening of charge gap

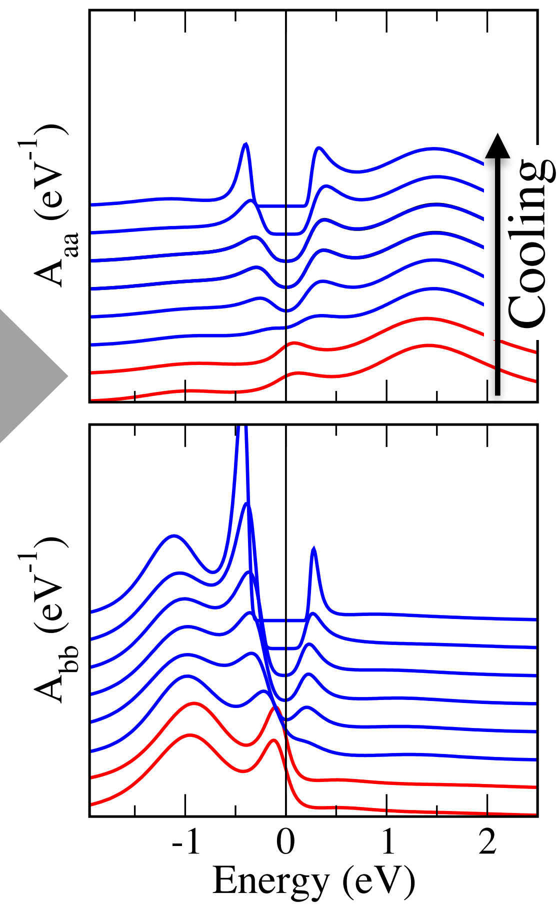
EC phase
(low T)



normal phase
(high T)

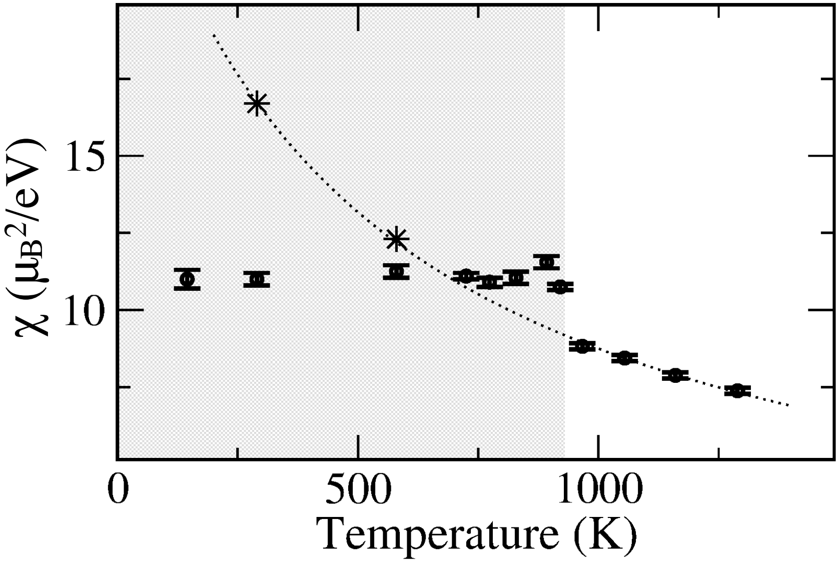


density (diagonal elements)

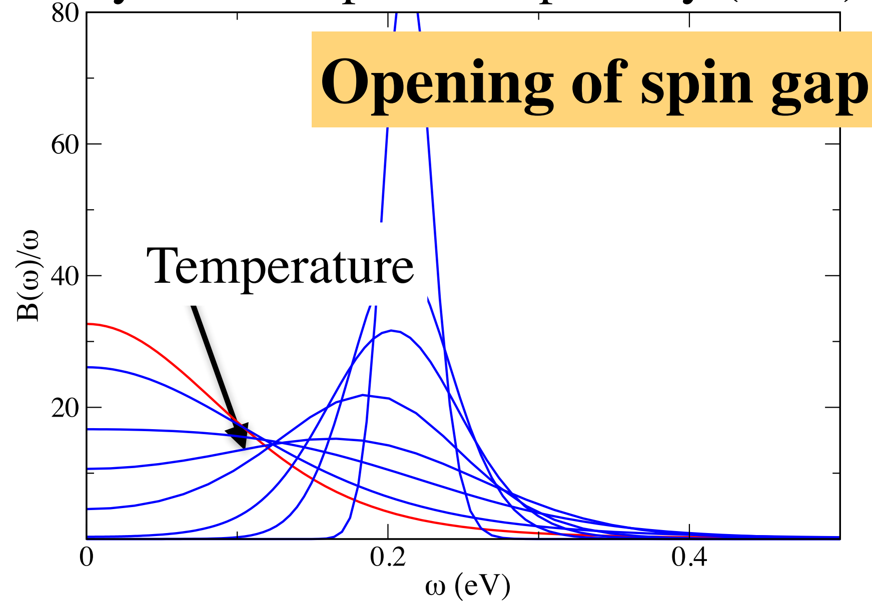


Undoped system - polar condensate

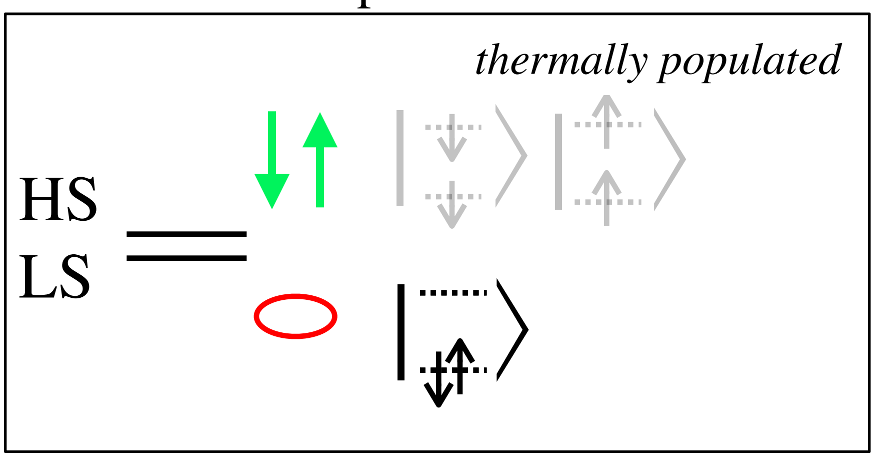
uniform spin susceptibility



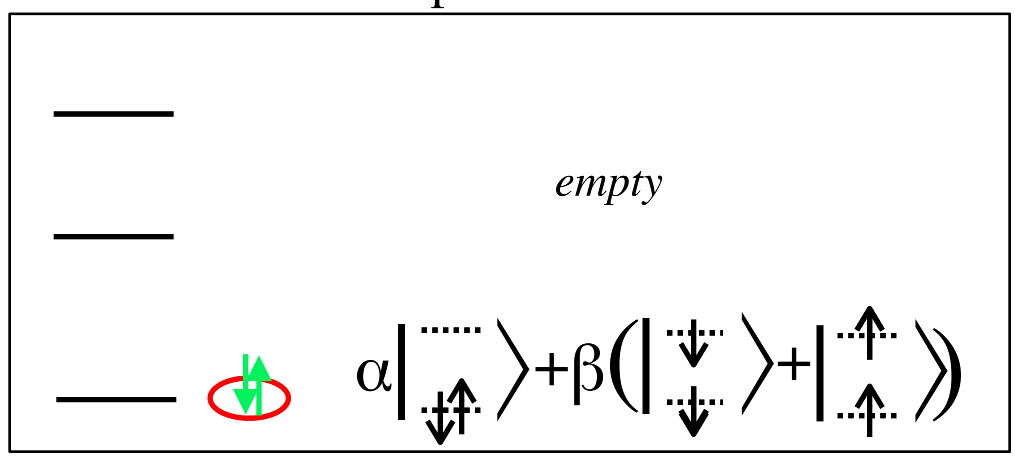
dynamical spin susceptibility (local)



atom in normal phase

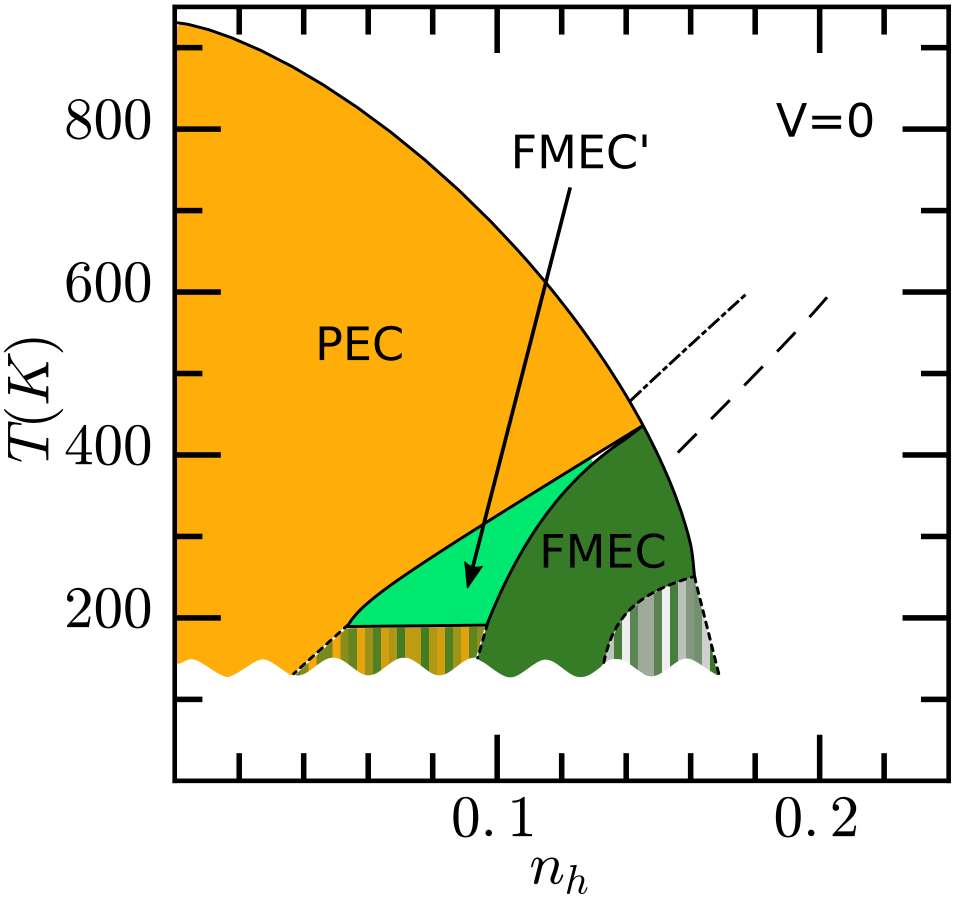


atom in condensed phase



Doping (no cross-hopping)

n-T phase diagram



Competition between
AFM super-exchange (PEC) and
double-exchange (FMEC)

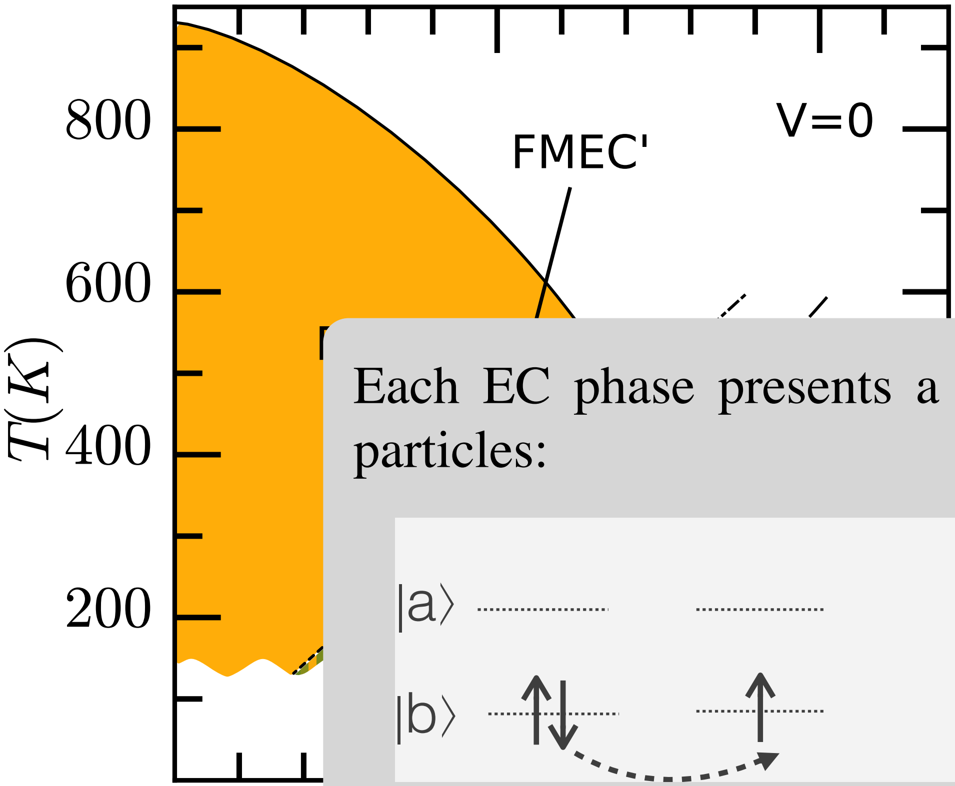
PEC - polar condensate $\overrightarrow{\phi} = \exp(i\varphi)\overrightarrow{x}$

FMEC - ferromagnetic condensate $\overrightarrow{M} = i\overrightarrow{\phi}^* \wedge \overrightarrow{\phi}$

Kuneš, 2014

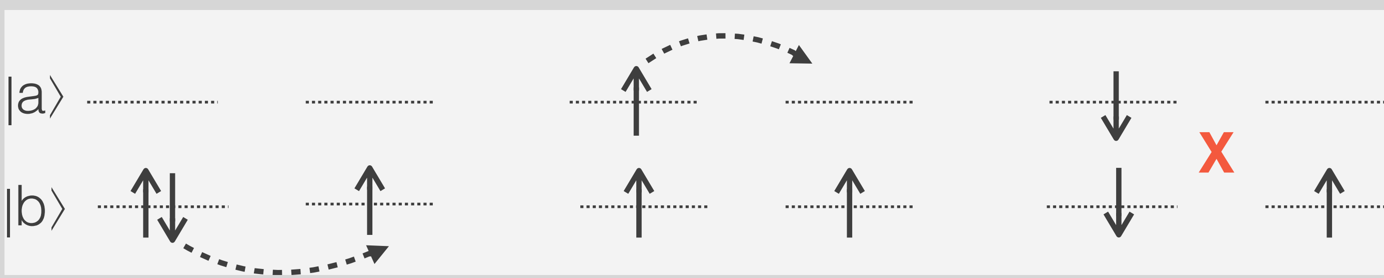
Doping (no cross-hopping)

n-T phase diagram



Competition between
AFM super-exchange (PEC) and
double-exchange (FMEC)

Each EC phase presents a distinct filter for propagation of doped particles:

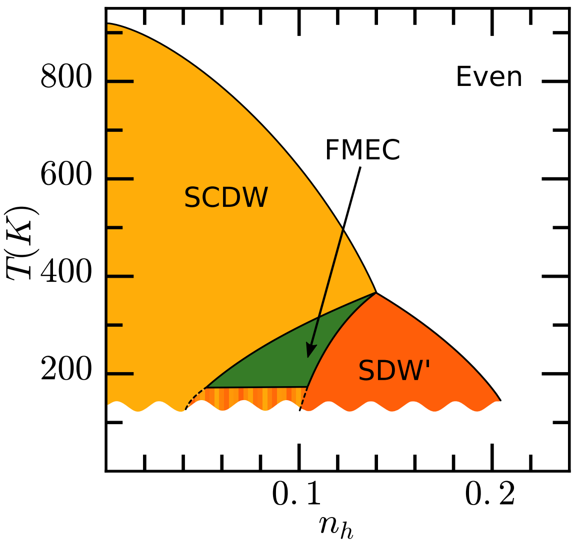


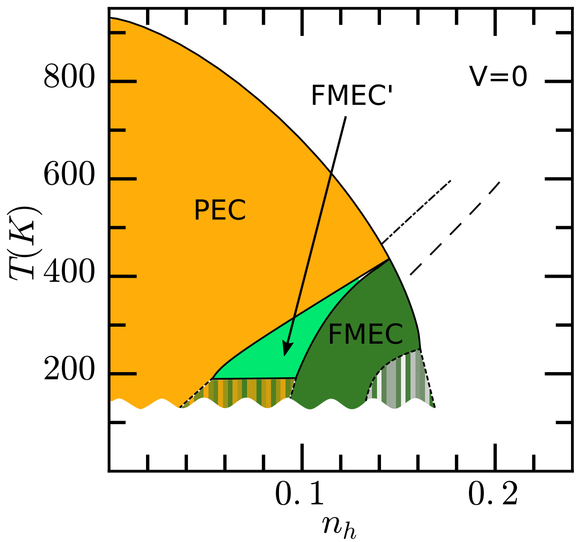
Stable phase is a result of competition between the kinetic energy of doped particles and super-exchange contribution to the condensation energy.

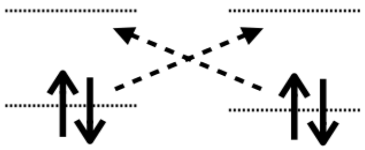
PEC - pola
FMEC - fe

Kuneš, 2014

Finite cross-hopping

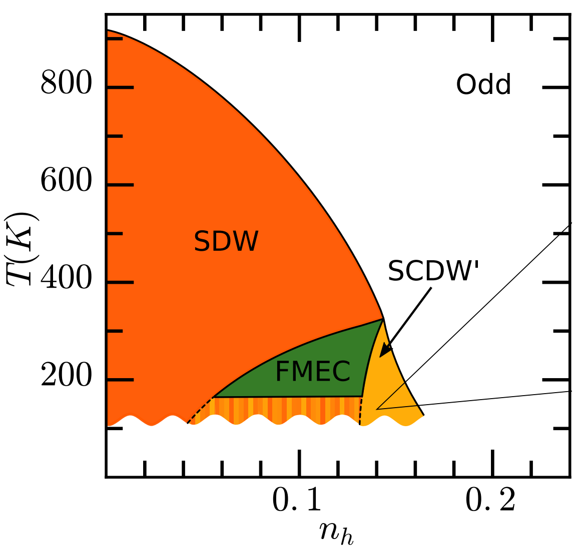






$V_1 = V_2$ even cross-hopping

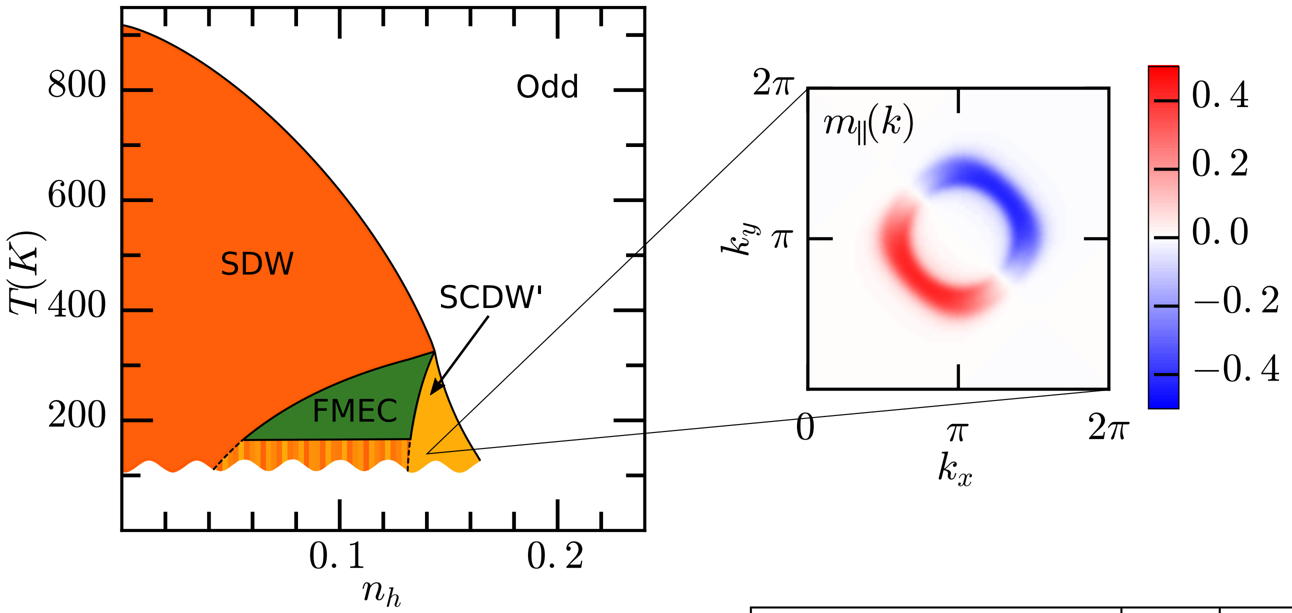
$V_1 = -V_2$ odd cross-hopping



Condensate state	$M_\perp$	$M_\parallel$	$\mathbf{m}(\mathbf{r})$	$\mathbf{m}_\mathbf{k}$	Re ϕ	Im ϕ
FMEC	✓	✓, 0	✓	✓	✓	✓
SDW	0	0	✓	0	✓	0
SCDW	0	0	0	0	0	✓
SDW'	0	✓	✓	✓	✓	0
SCDW'	0	0	0	✓	0	✓

PEC
- SDW $\overrightarrow{\phi} = \overrightarrow{x}$
- SCDW $\overrightarrow{\phi} = i\,\overrightarrow{x}$

Spin texture

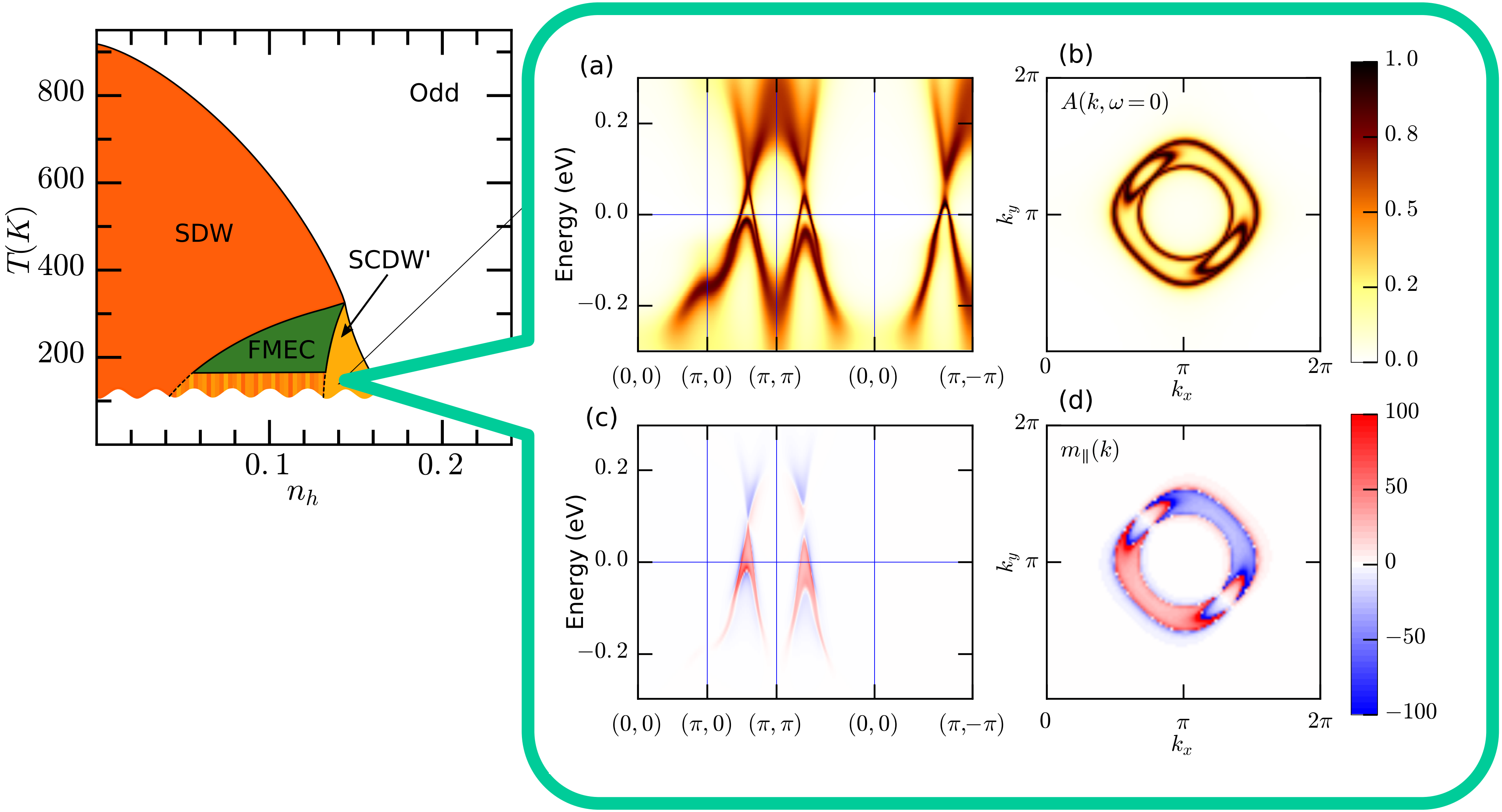


Condensate state	$M_\perp$	$M_\parallel$	$\mathbf{m}(\mathbf{r})$	$\mathbf{m}_\mathbf{k}$	Re ϕ	Im ϕ
FMEC	✓	✓, 0	✓	✓	✓	✓
SDW	0	0	✓	0	✓	0
SCDW	0	0	0	0	0	✓
SDW’	0	✓	✓	✓	✓	0
SCDW’	0	0	0	✓	0	✓

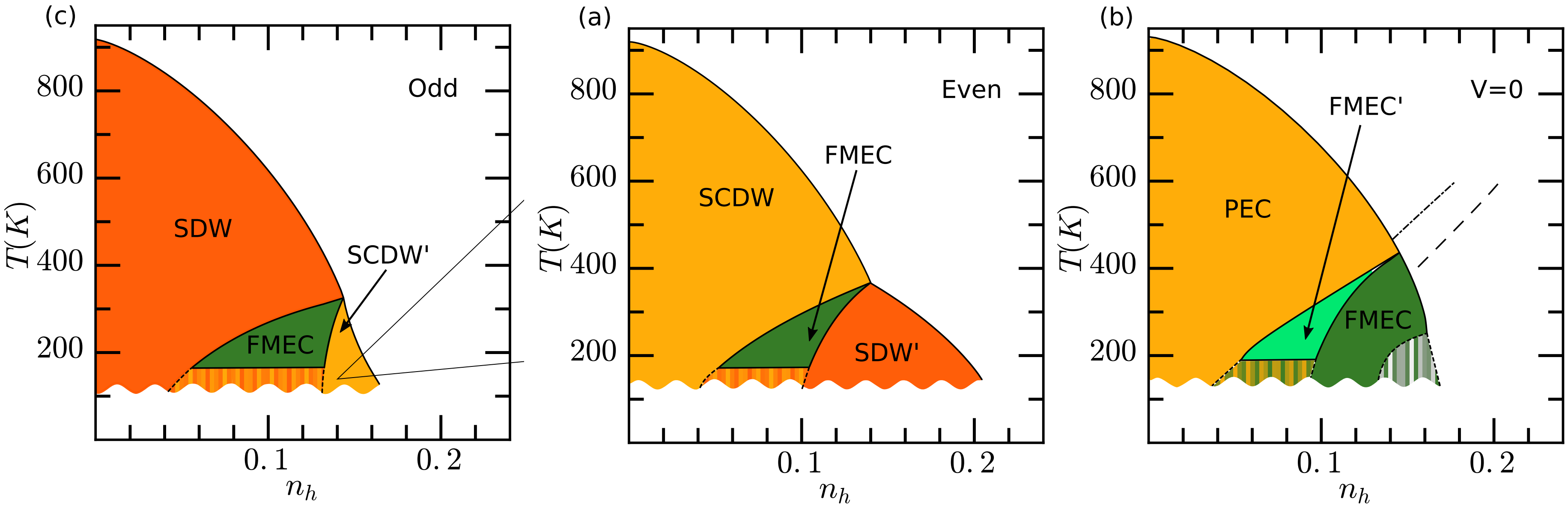
Dynamically generated Dresselhaus-Rashba spin-orbit coupling

centrosymmetric Hamiltonian, no spin-orbit coupling

Spin texture



Spin texture



Effective model for propagation of doped fermions:

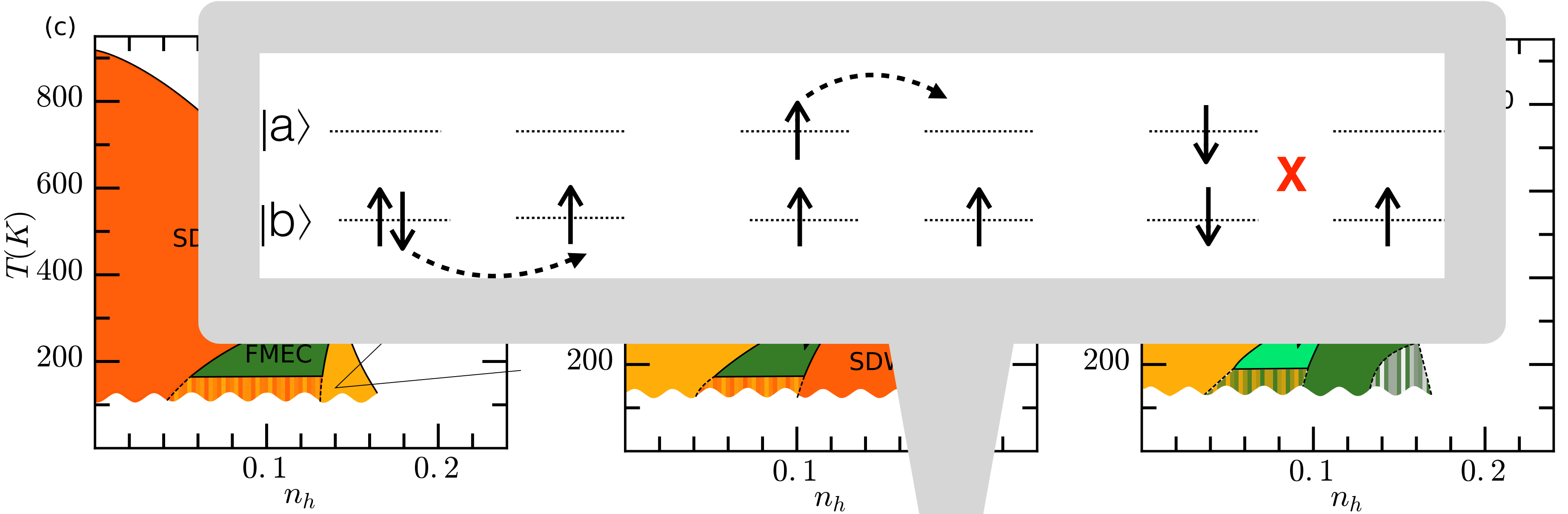
$$H_{\rm eff} = \sum_{\langle ij \rangle} \bar{h}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta} + \text{h.c.}$$

$$\bar{h} = t_s \bar{I} - \frac{i t_a}{4 s^2} (\boldsymbol{\phi}^* \wedge \boldsymbol{\phi}) \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{2} (V_1 \boldsymbol{\phi} + V_2 \boldsymbol{\phi}^*) \cdot \bar{\boldsymbol{\sigma}}$$

$$\bar{h}_{\mathbf{k}} = 2 t_s \bar{I} C_{\mathbf{k}} + 2 V_1 \boldsymbol{\phi} \cdot \bar{\boldsymbol{\sigma}} \begin{cases} C_{\mathbf{k}} & \text{SDW'} \\ i S_{\mathbf{k}} & \text{CSDW'} \end{cases}$$

with $\quad C_{\mathbf{k}} = \cos k_x + \cos k_y, \quad S_{\mathbf{k}} = \sin k_x + \sin k_y.$

Spin texture



Effective model for propagation of doped fermion

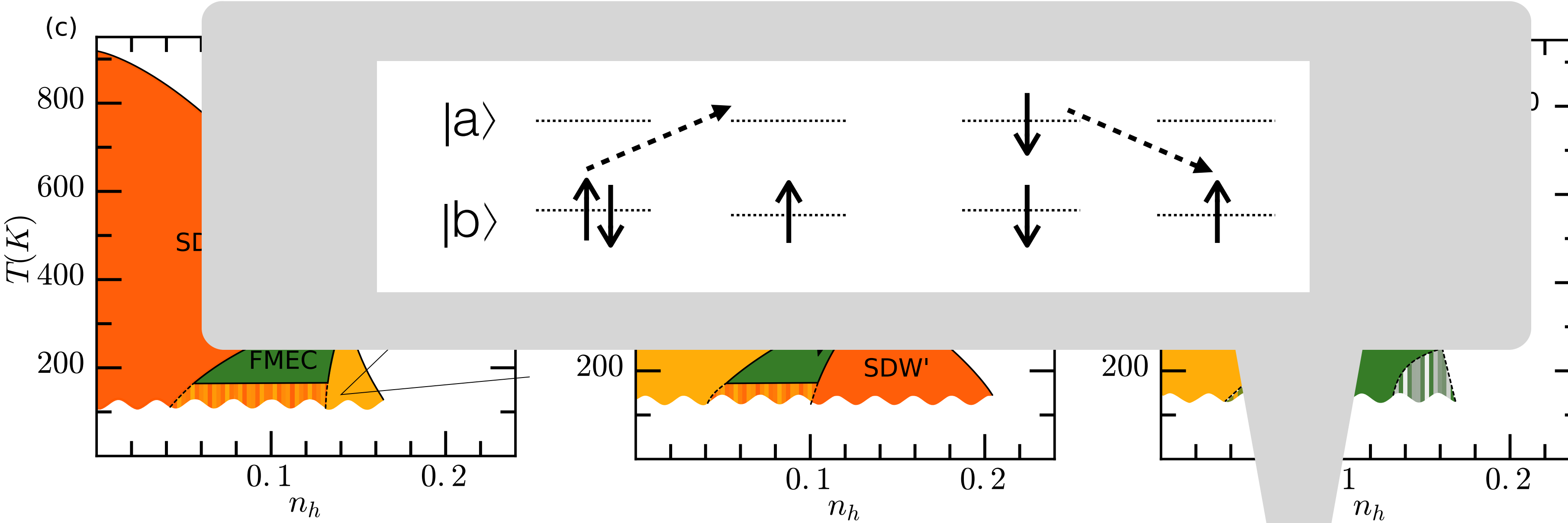
$$H_{\text{eff}} = \sum_{\langle ij \rangle} \bar{h}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta} + \text{h.c.}$$

$$\bar{h} = t_s \bar{I} - \frac{i t_a}{4s^2} (\boldsymbol{\phi}^* \wedge \boldsymbol{\phi}) \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{2} (V_1 \boldsymbol{\phi} + V_2 \boldsymbol{\phi}^*) \cdot \bar{\boldsymbol{\sigma}}$$

$$\bar{h}_{\mathbf{k}} = 2 t_s \bar{I} C_{\mathbf{k}} + 2 V_1 \boldsymbol{\phi} \cdot \bar{\boldsymbol{\sigma}} \begin{cases} C_{\mathbf{k}} & \text{SDW'} \\ i S_{\mathbf{k}} & \text{CSDW'} \end{cases}$$

with $\quad C_{\mathbf{k}} = \cos k_x + \cos k_y, \quad S_{\mathbf{k}} = \sin k_x + \sin k_y.$

Spin texture



Effective model for propagation of doped fermions:

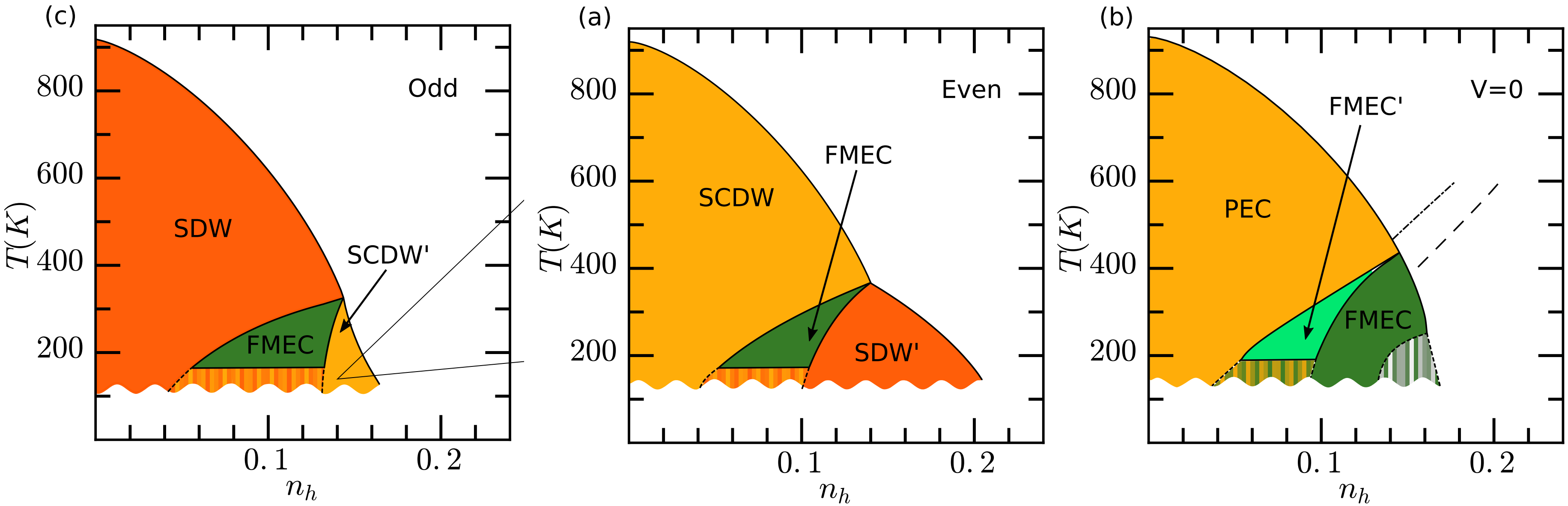
$$H_{\rm eff} = \sum_{\langle ij \rangle} \bar{h}_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta} + \text{h.c.}$$

$$\bar{h} = t_s \bar{I} - \frac{i t_a}{4s^2} (\boldsymbol{\phi}^* \wedge \boldsymbol{\phi}) \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{2} (V_1 \boldsymbol{\phi} + V_2 \boldsymbol{\phi}^*) \cdot \bar{\boldsymbol{\sigma}}$$

$$\bar{h}_{\mathbf{k}} = 2 t_s \bar{I} C_{\mathbf{k}} + 2 V_1 \boldsymbol{\phi} \cdot \bar{\boldsymbol{\sigma}} \begin{cases} C_{\mathbf{k}} & \text{SDW'} \\ i S_{\mathbf{k}} & \text{CSDW'} \end{cases}$$

with $\quad C_{\mathbf{k}} = \cos k_x + \cos k_y, \quad S_{\mathbf{k}} = \sin k_x + \sin k_y.$

Spin texture



Effective model for propagation of doped fermions:

$$H_{\text{eff}} = \sum_{\langle ij \rangle} \bar{h}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta} + \text{h.c.}$$

$$\bar{h} = t_s \bar{I} - \frac{i t_a}{4 s^2} (\boldsymbol{\phi}^* \wedge \boldsymbol{\phi}) \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{2} (V_1 \boldsymbol{\phi} + V_2 \boldsymbol{\phi}^*) \cdot \bar{\boldsymbol{\sigma}}$$

$$\bar{h}_{\mathbf{k}} = 2 t_s \bar{I} C_{\mathbf{k}} + 2 V_1 \boldsymbol{\phi} \cdot \bar{\boldsymbol{\sigma}} \begin{cases} C_{\mathbf{k}} & \text{SDW'} \\ i S_{\mathbf{k}} & \text{CSDW'} \end{cases}$$

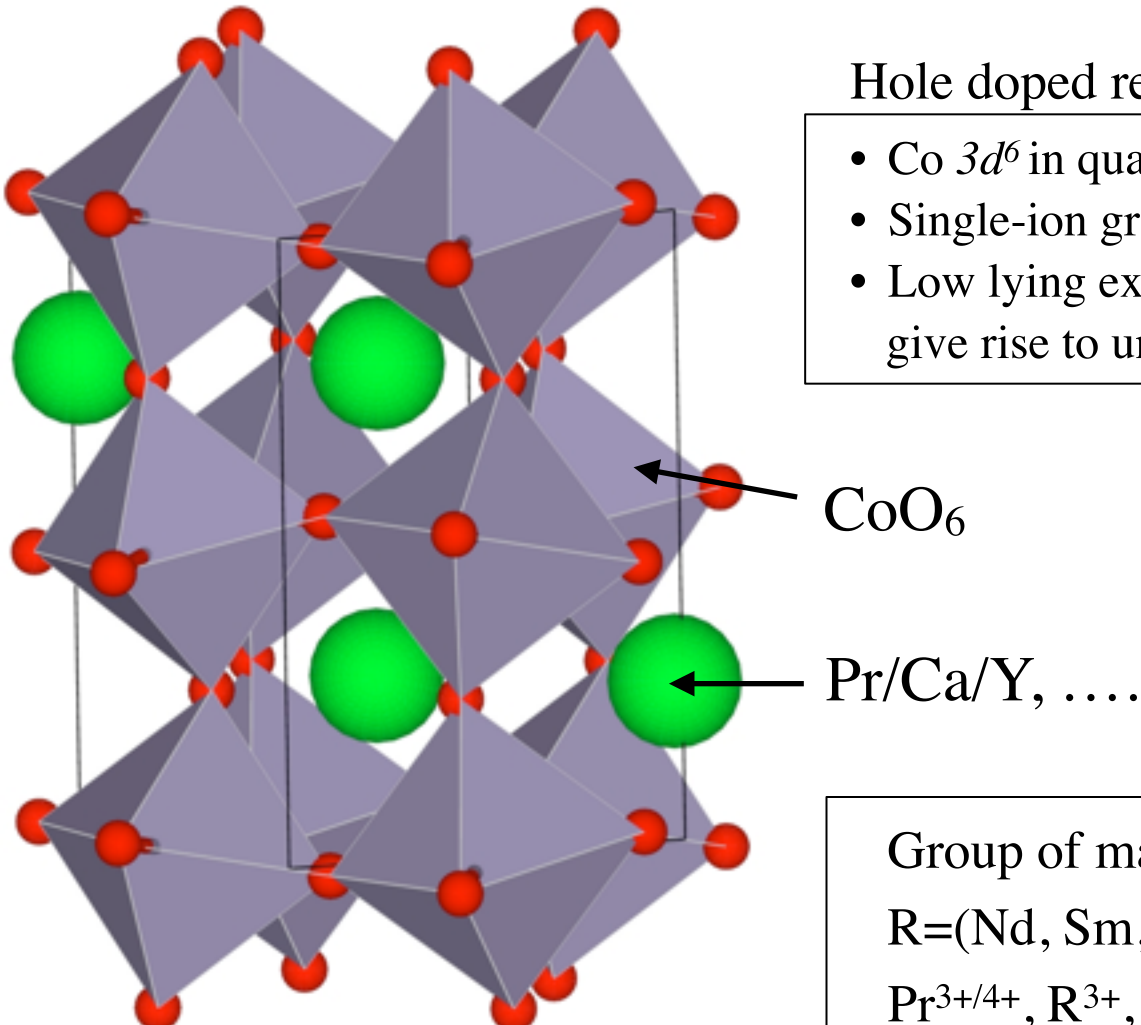
with $\quad C_{\mathbf{k}} = \cos k_x + \cos k_y, \quad S_{\mathbf{k}} = \sin k_x + \sin k_y.$

The puzzle of PCCO

Immanuel Kant

"Experience without theory is blind, but theory without experience is mere intellectual play."

$Pr_{0.5}Ca_{0.5}CoO_3$ (PCCO)



Hole doped relative of **$LaCoO_3$**

- Co *$3d^6$* in quasi-cubic crystal field
- Single-ion ground state is singlet (LS)
- Low lying excited multiplets S=1 or S=2 give rise to unusual magnetic response

Group of materials: $(Pr_{1-y}R_y)_{1-x}Ca_xCoO_3$

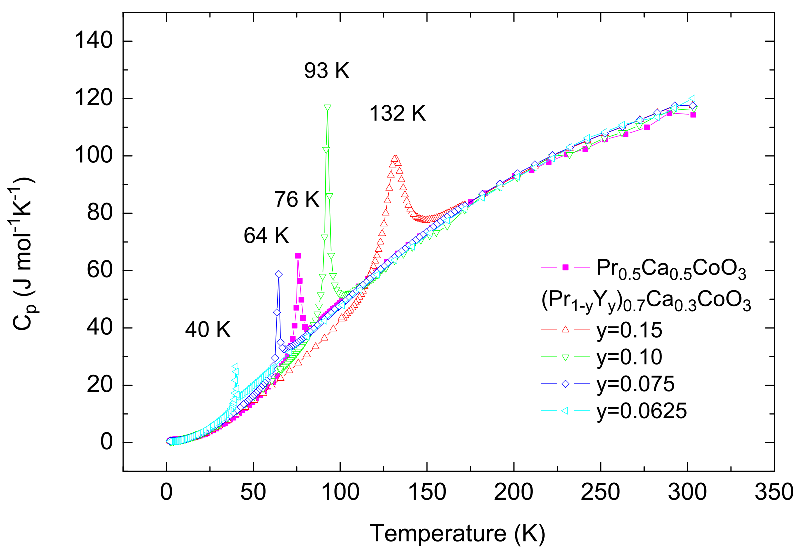
R=(Nd, Sm, Eu, Gd, Tb, Y)

$Pr^{3+/4+}$, R^{3+}, Ca^{2+}, Co^{3+}, O^{2-}

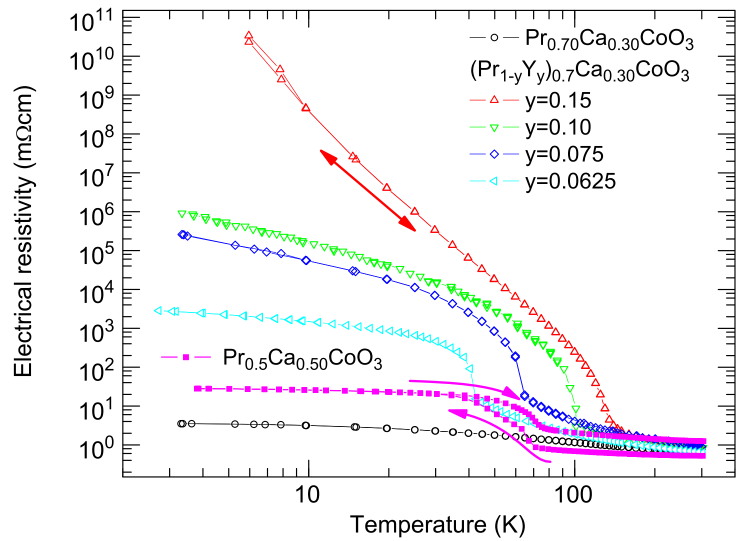
avg. valence at low T is close to A^{3+}

$Pr_{0.5}Ca_{0.5}CoO_3$ (PCCO)

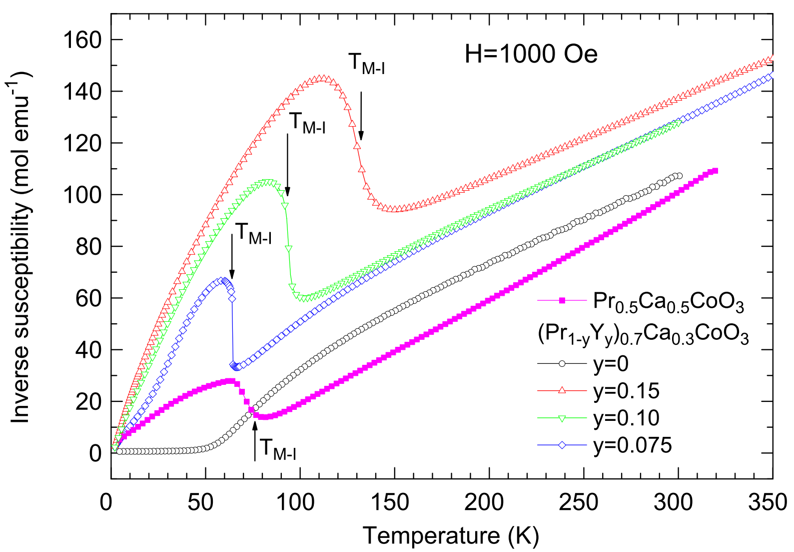
specific heat:



resistivity:



inverse susceptibility:

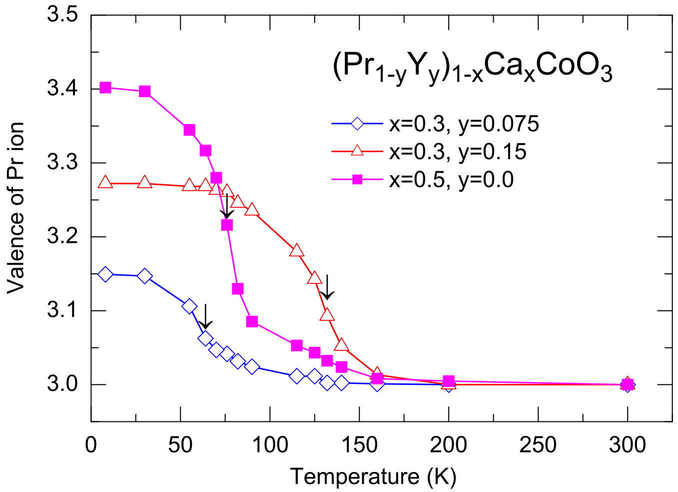


1. continuous phase transition
2. metal-insulator transition
3. drop of magnetic susceptibility

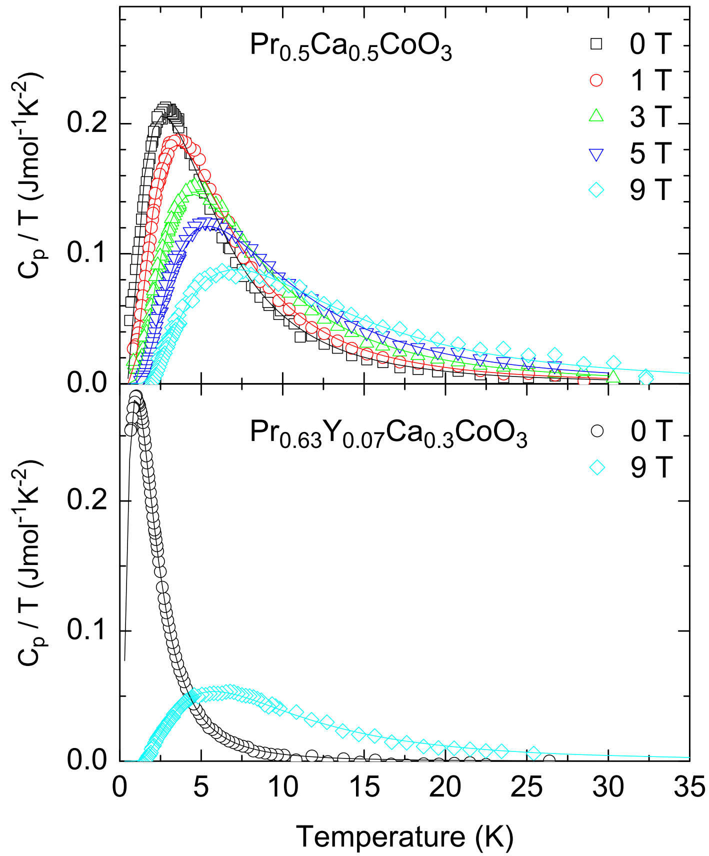
Tsubouchi et al., 2002
Hejtmánek et al., 2013

$Pr_{0.5}Ca_{0.5}CoO_3$ (PCCO)

Pr^{3+}->Pr^{4+} valence transition:



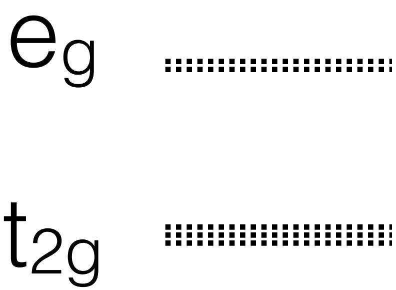
Pr^{4+} Schottky peak:



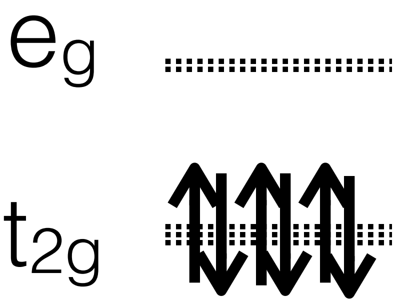
4. Pr^{3+}->Pr^{4+} valence transition
5. exchange splitting of Pr^{4+} ground state, but no magnetic order detected

Hejtmánek et al., 2013

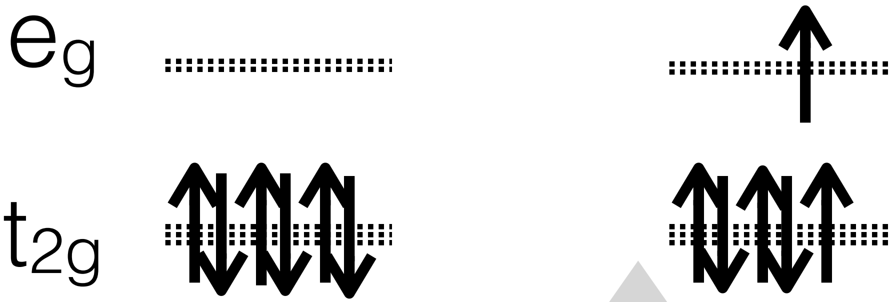
Excitonic condensation in cubic d^6 perovskite



Excitonic condensation in cubic d^6 perovskite

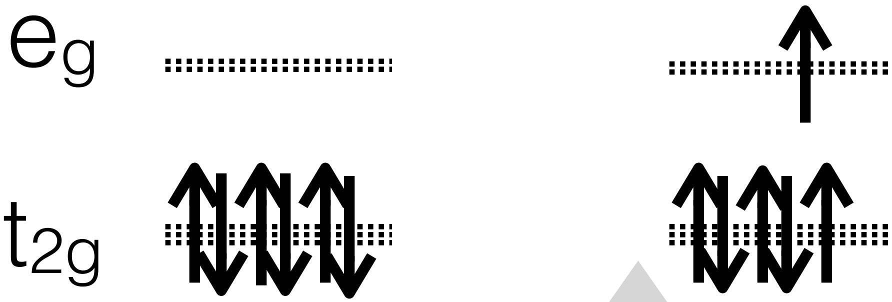


Excitonic condensation in cubic d^6 perovskite



Exciton = bound pair of e_g electron and t_{2g} hole

Excitonic condensation in cubic d^6 perovskite

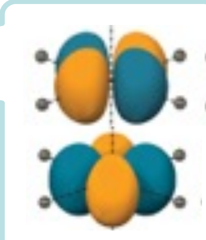


Orbital degeneracy

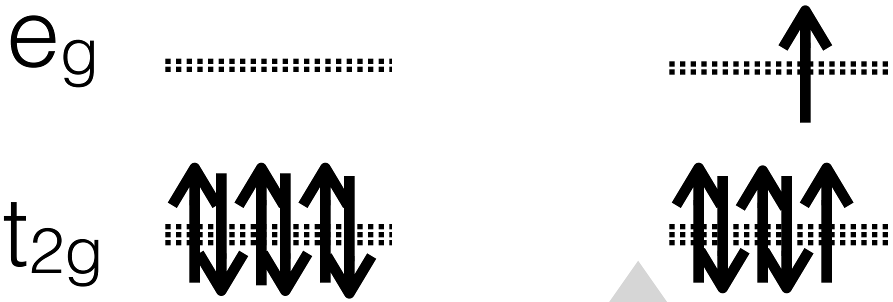
Exciton = bound pair of e_g electron and t_{2g} hole

T_{1g} exciton:

$$d_{x^2-y^2} \otimes d_{xy}$$
$$d_{z^2-x^2} \otimes d_{zx}$$
$$d_{y^2-z^2} \otimes d_{yz}$$



Excitonic condensation in cubic d^6 perovskite



Orbital degeneracy

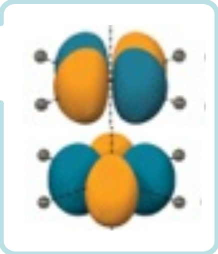
Exciton = bound pair of e_g electron and t_{2g} hole

T_{1g} exciton:

$d_{x^2-y^2} \otimes d_{xy}$

$d_{z^2-x^2} \otimes d_{zx}$

$d_{y^2-z^2} \otimes d_{yz}$



The order parameter has 9 components (or 18 real components)

ϕ_β^α

$\alpha = x, y, z$ transforms like a vector under spin rotations

$\beta = xy, zx, yz$ transforms like a pseudovector under O_h operations

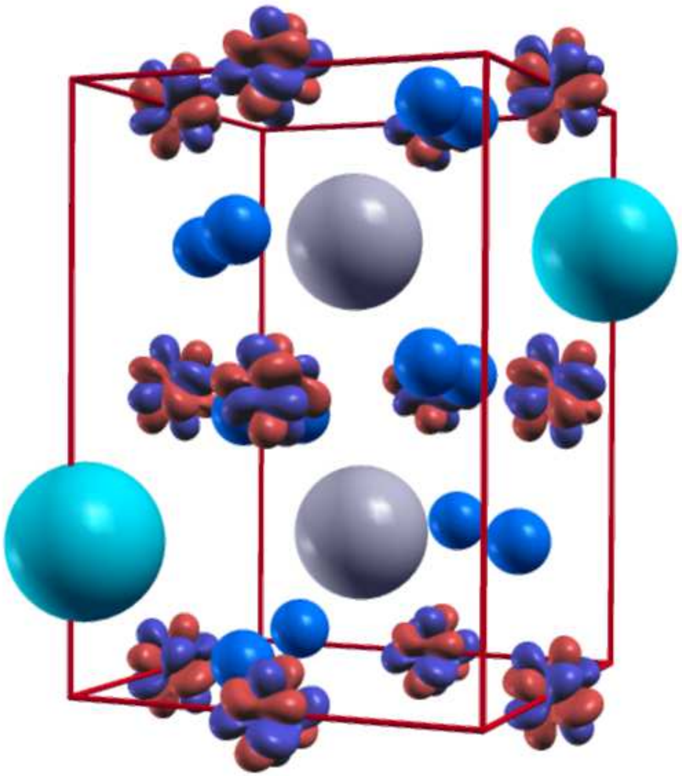
Many phases possible - oder a parameter is similar to ^{3}He

Bruder and Vollhardt, 1986

Origin of exchange splitting on Pr (LDA+U)

Coupling of Pr 4f[1] spin to p-d orbitals: effective multi-channel Kondo Hamiltonian

$$H^{(n)} = \sum_{\alpha\alpha'} \sum_{mm'} \sum_{i} \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\alpha'} J^{(n)}_{i,mm'} c^{\dagger}_{im\alpha} c_{im'\alpha'} + \text{c.c.}$$

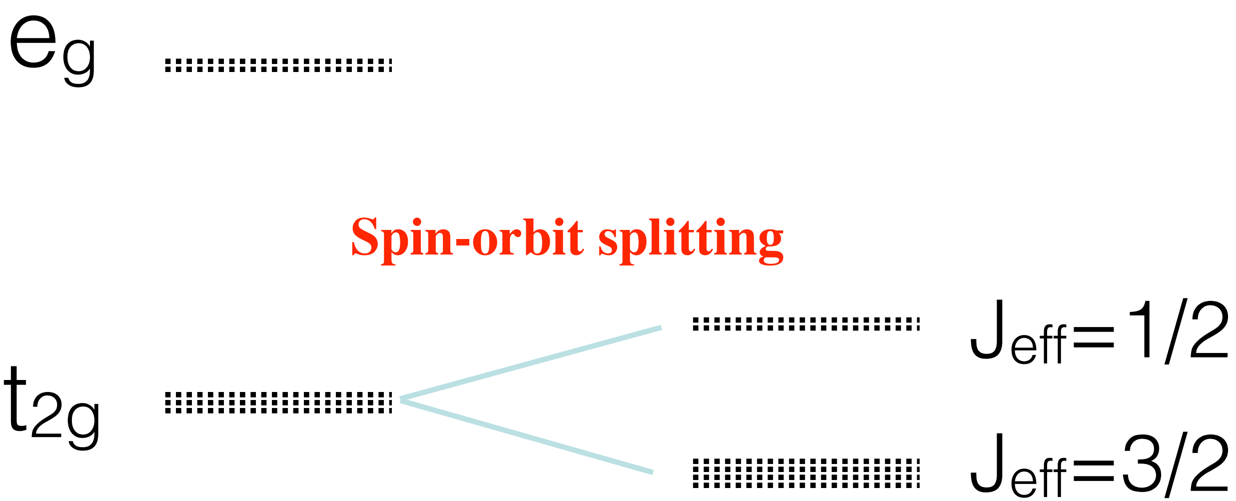


Below T_c effective exchange field appears:

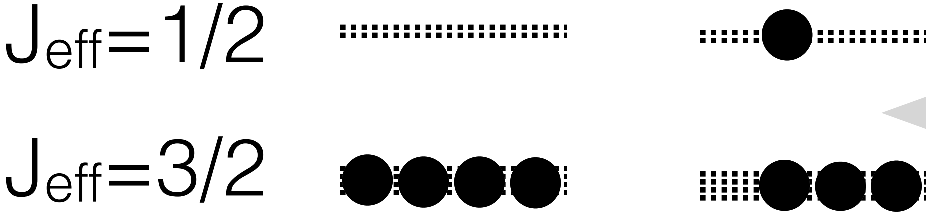
$$h^{(n)}_{\gamma} = \sum_{imm'} J^{(n)}_{i,mm'} \sum_{\alpha\alpha'} 2\,\mathrm{Re}\langle c^{\dagger}_{im\alpha} \sigma^{\gamma}_{\alpha\alpha'} c_{im'\alpha'} \rangle$$

Kuneš and Augustinský, 2014

Cubic d^4 perovskite with strong spin-orbit coupling



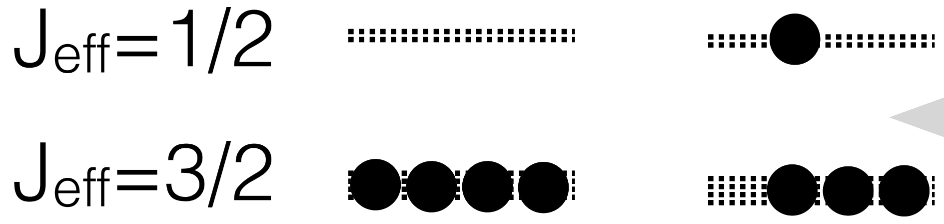
Cubic d^4 perovskite with strong spin-orbit coupling



Exciton = bound pair of $j_{1/2}$ electron and $j_{3/2}$ hole

Khaliullin, 2013

Cubic d^4 perovskite with strong spin-orbit coupling

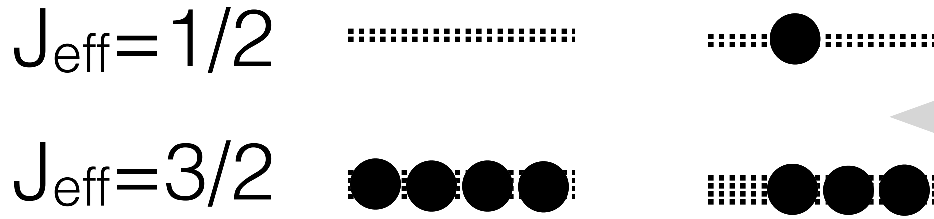


Exciton = bound pair of $j_{1/2}$ electron and $j_{3/2}$ hole

Khaliullin, 2013

Double-perovskites Ba_2YIrO_6 and Sr_2YIrO_6 ? (exp) *Cao et al., 2014*

Cubic d^4 perovskite with strong spin-orbit coupling

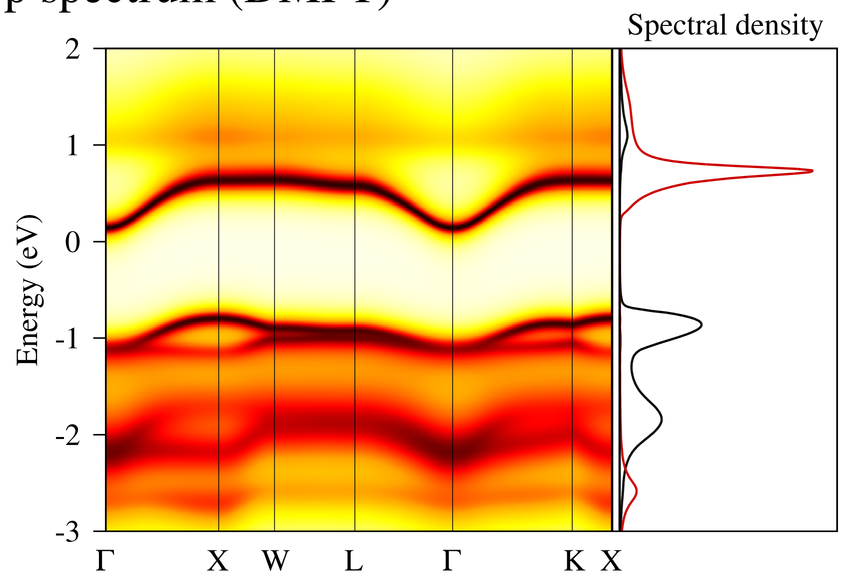


Exciton = bound pair of $j_{1/2}$ electron and $j_{3/2}$ hole

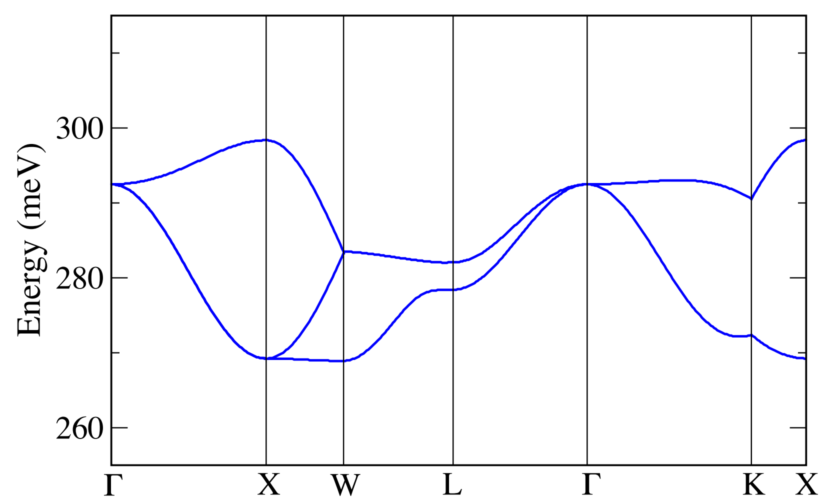
Khaliullin, 2013

Double-perovskites Ba_2YIrO_6 and Sr_2YIrO_6 ? (exp) *Cao et al., 2014*

1-p spectrum (DMFT)



2-p spectrum (strong-coupling expansion)



No excitonic magnetism! *Pajskr et al., 2013*

Conclusions

- Solids close to **spin-state transition** may be unstable towards **condensation of spinful excitons**.

- Excitonic condensation can give rise to **number of phases** with rather diverse properties.

- **Doping** activates generalised double-exchange mechanism with interesting consequences (e.g. spontaneous spin texture)

- There are some promising materials - PCCO.

Phys. Rev. B **89**, 115134 (2014)
Phys. Rev. B **90**, 235112 (2014)
Phys. Rev. B **90**, 235140 (2014)
J. Phys.: Condensed. Matter **27**, 333201 (2015) - Topical Review
Phys. Rev. B **93**, 035129 (2016)
arXiv:1602.07122